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# A Water-Mediated and Substrate-Assisted Aminoacylation Mechanism in the Discriminating Aminoacyl-tRNA Synthetase GlnRS and Non-Discriminating GluRS

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**Supporting Information**

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## Figures

**Figure S1.** Overlay of the active site of GlnRS after MD (grey) with the crystal structure 1EUQ (turquoise).

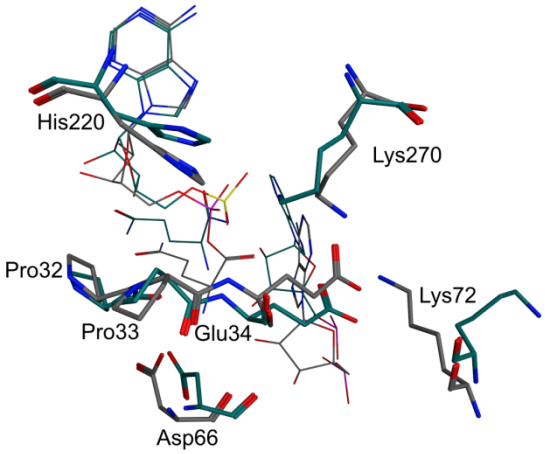



**Figure S2.** Overlay of the active site of GlnRS after MD (grey) with the crystal structure 1EUQ (turquoise).

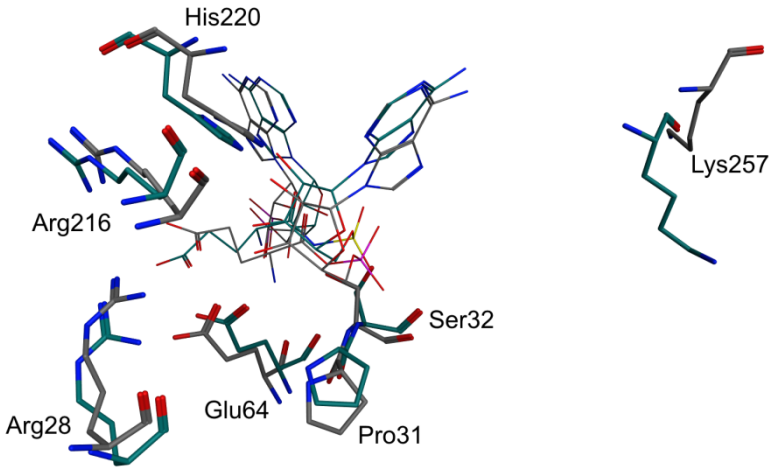


**Figure S3**. Overlay of structures from MD simulations of GlnRS (grey) and ND-GluRS (green) showing position of key lysine residues and the structural Glu34 residue.

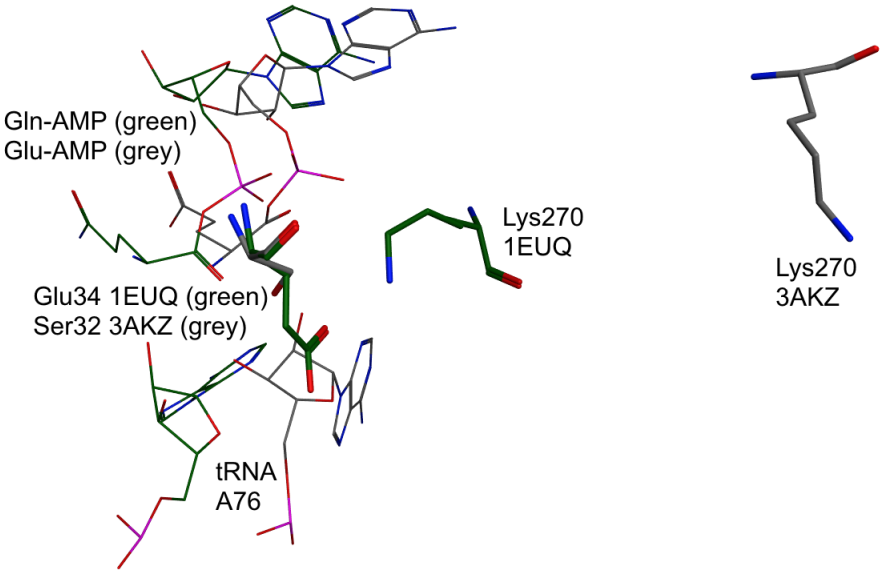



**Figure S4**. Plot of the calculated RMSD for the GlnRS enzyme over the course of a 10 ns MD simulation.

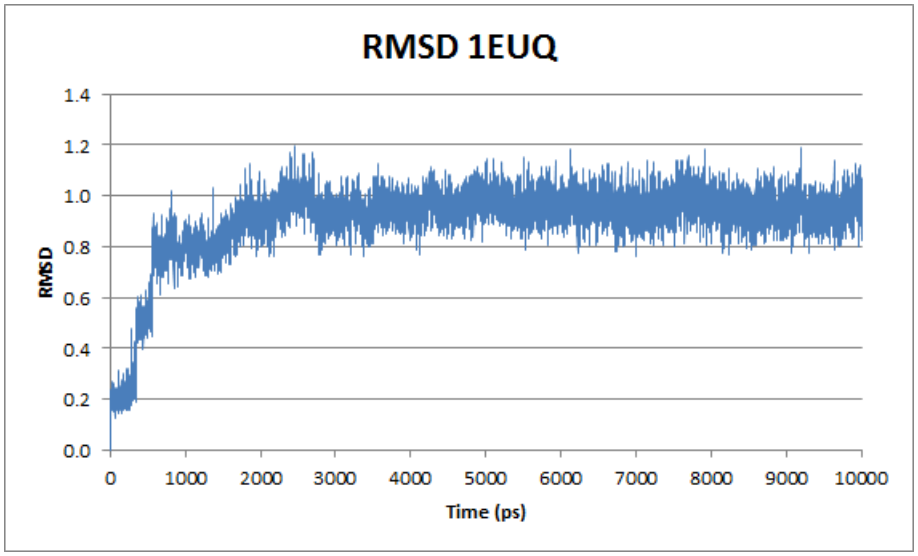
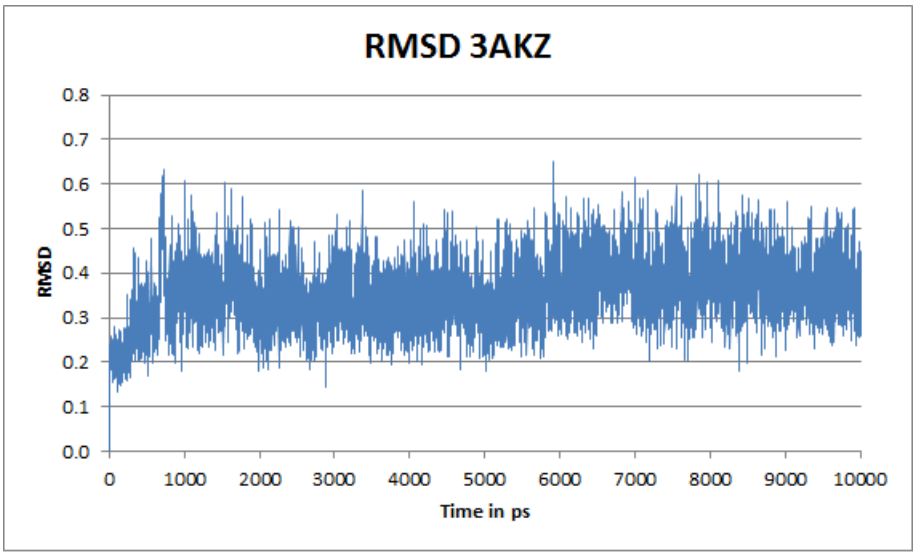


**Figure S5**. Plot of the calculated RMSD for the ND-GluRS enzyme over the course of a 10 ns MD simulation.



# Tables of Coordinates

## GlnRS

**Table S1.** Cartesian coordinates and partial charges of all GlnRS species presently optimized using the ONIOM(QM/MM) approach.

**RC**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.48288 | -11.75722 | -5.5125 | L |
| C-C-0.597200 | 0 | -11.8062 | -10.73972 | -6.40177 | L |
| O-O--0.567900 | 0 | -11.41632 | -11.09027 | -7.50669 | L |
| H-HC-0.112300 | 0 | -11.87794 | -11.90667 | -4.62104 | L |
| H-HC-0.112300 | 0 | -12.56429 | -12.69577 | -6.05858 | L |
| H-HC-0.112300 | 0 | -13.47577 | -11.39785 | -5.25132 | L |
| N-N--0.415700 | 0 | -11.63672 | -9.51444 | -5.89565 | L |
| C-CT--0.058100 | -1 | -10.78 | -8.48167 | -6.49788 | L |
| C-C-0.597300 | 0 | -9.75845 | -7.95724 | -5.48306 | L |
| O-O--0.567900 | 0 | -10.03398 | -7.88962 | -4.27883 | L |
| C-CT--0.007400 | 0 | -11.59339 | -7.38649 | -7.18236 | L |
| C-CC-0.186800 | 0 | -10.9947 | -6.90422 | -8.47743 | L |
| N-NB--0.543200 | 0 | -11.38679 | -7.31641 | -9.75073 | L |
| C-CW--0.220700 | 0 | -10.12749 | -5.86095 | -8.59285 | L |
| C-CR-0.163500 | 0 | -10.80098 | -6.46177 | -10.60226 | L |
| N-NA--0.279500 | 0 | -10.04214 | -5.57681 | -9.93692 | L |
| H-H-0.271900 | 0 | -12.00975 | -9.3133 | -4.98379 | L |
| H-H1-0.136000 | 0 | -10.2073 | -8.96938 | -7.28896 | L |
| H-HC-0.036700 | 0 | -11.65977 | -6.53713 | -6.51212 | L |
| H-HC-0.036700 | 0 | -12.60143 | -7.74614 | -7.39348 | L |
| H-H4-0.186200 | 0 | -9.70535 | -5.283 | -7.7859 | L |
| H-H-0.333900 | 0 | -9.69506 | -4.69769 | -10.34002 | L |
| H-H5-0.143500 | 0 | -10.9787 | -6.43589 | -11.66791 | L |
| N-N--0.415700 | 0 | -8.56861 | -7.61385 | -5.97042 | L |
| C-CT--0.038900 | -1 | -7.41237 | -7.10423 | -5.21183 | L |
| C-C-0.597300 | 0 | -6.64627 | -6.01992 | -6.00629 | L |
| O-O--0.567900 | 0 | -6.99172 | -5.71681 | -7.14787 | L |
| C-CT-0.365400 | 0 | -6.41757 | -8.22951 | -4.85717 | L |
| O-OH--0.676100 | 0 | -6.13203 | -9.01222 | -5.97752 | L |
| C-CT--0.243800 | -1 | -6.92337 | -9.17353 | -3.78364 | L |
| H-H-0.271900 | 0 | -8.41491 | -7.80535 | -6.95435 | L |
| H-H1-0.100700 | 0 | -7.74111 | -6.67401 | -4.27349 | L |
| H-H1-0.004300 | 0 | -5.48863 | -7.79355 | -4.48951 | L |
| H-HC-0.064200 | 0 | -7.19878 | -8.60707 | -2.89393 | L |
| H-HC-0.064200 | 0 | -6.14091 | -9.88465 | -3.52348 | L |
| H-HC-0.064200 | 0 | -7.79727 | -9.71431 | -4.14783 | L |
| H-HO-0.410200 | 0 | -5.41346 | -9.63046 | -5.76784 | L |
| N-N--0.347900 | 0 | -5.57584 | -5.43145 | -5.43685 | L |
| C-CT--0.263700 | -1 | -4.59362 | -4.5803 | -6.15736 | L |
| C-C-0.734100 | 0 | -3.1902 | -4.64107 | -5.56746 | L |
| O-O--0.589400 | 0 | -3.06321 | -4.87922 | -4.37199 | L |
| C-CT--0.000700 | 0 | -5.09331 | -3.12686 | -6.26852 | L |

```
 C-CT-0.039000        0    -4.86497  -2.21837  -5.04669  L
 C-CT-0.048600        0    -5.67197  -2.54265  -3.78887  L
 N-N2--0.529500       0    -5.06031  -3.58809  -2.96304  L
 C-CA-0.807600        0    -5.04419  -3.65459  -1.65164  L
 N-N2--0.862700       0    -5.73952  -2.88093  -0.87305  L
 N-N2--0.862700       0    -4.27797  -4.54257  -1.10235  L
 H-H-0.274700         0    -5.34686  -5.72603  -4.49958  L
 H-H1-0.156000        0    -4.53373  -4.98533  -7.16397  L
 H-HC-0.032700        0    -6.15352  -3.12093  -6.52645  L
 H-HC-0.032700        0    -4.56761  -2.66734  -7.10692  L
 H-HC-0.028500        0    -5.16485  -1.22328  -5.34571  L
 H-HC-0.028500        0    -3.8061   -2.16301  -4.80243  L
 H-H1-0.068700        0    -6.68098  -2.83094  -4.079    L
 H-H1-0.068700        0    -5.71832  -1.62616  -3.19896  L
 H-H-0.345600         0    -4.40807  -4.20625  -3.42156  L
 H-H-0.447800         0    -5.77755  -2.99757   0.12848  L
 H-H-0.447800         0    -6.48167  -2.29192  -1.27592  L
 H-H-0.447800         0    -3.98076  -4.38857  -0.14519  L
 H-H-0.447800         0    -3.83279  -5.24844  -1.68015  L
 N-N--0.415700        0    -2.14719  -4.31251  -6.32331  L
 C-CT--0.002400      -1    -0.90457  -3.79393  -5.7281   L
 C-C-0.597300         0    -0.97015  -2.25629  -5.66992  L
 O-O--0.567900        0    -1.11158  -1.6487   -6.73505  L
 C-CT--0.034300       0     0.31485  -4.26889  -6.52757  L
 C-CA-0.011800        0     1.62487  -3.67821  -6.03055  L
 C-CA--0.125600       0     2.09027  -3.95301  -4.72827  L
 C-CA--0.125600       0     2.3717   -2.8268   -6.86572  L
 C-CA--0.170400       0     3.27764  -3.35531  -4.26435  L
 C-CA--0.170400       0     3.55046  -2.22283  -6.39895  L
 C-CA--0.107200       0     3.99286  -2.47071  -5.09101  L
 H-H-0.271900         0    -2.34543  -4.15112  -7.30658  L
 H-H1-0.097800        0    -0.7831   -4.19902  -4.72598  L
 H-HC-0.029500        0     0.17437  -4.00381  -7.57698  L
 H-HC-0.029500        0     0.37669  -5.35566  -6.45998  L
 H-HA-0.133000        0     1.53413  -4.61472  -4.079    L
 H-HA-0.133000        0     2.02938  -2.61175  -7.86465  L
 H-HA-0.143000        0     3.63857  -3.56434  -3.26833  L
 H-HA-0.143000        0     4.10672  -1.55362  -7.04024  L
 H-HA-0.129700        0     4.88254  -1.97324  -4.73091  L
 N-N--0.254800        0    -0.91095  -1.63499  -4.47132  L
 C-CT--0.026600       0    -1.05386  -0.18921  -4.30538  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.27743   0.54666  -3.96956  H
 O-O--0.574800        0     0.67189   0.67473  -2.81872  H
 C-CT--0.007000       0    -2.07167  -0.07448  -3.16594  L
 C-CT-0.018900        0    -1.68401  -1.2209   -2.23331  L
 C-CT-0.019200        0    -1.1407   -2.28674  -3.18223  L
 H-H1-0.064100        0    -1.49243   0.25296  -5.18991  L
 H-HC-0.025300        0    -3.07792  -0.23643  -3.55318  L
 H-HC-0.025300        0    -2.02107   0.8808   -2.65545  L
 H-HC-0.021300        0    -2.54377  -1.58308  -1.66842  L
```

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 H-HC-0.021300        0    -0.89498  -0.90379  -1.55579  L
 H-H1-0.039100        0    -0.21412  -2.70677  -2.79074  L
 H-H1-0.039100        0    -1.89394  -3.06457  -3.27409  L
 N-N--0.254800        0     0.98315   1.10356  -5.00403  H
 C-CT--0.026600       0     2.15403   1.923    -4.71262  H
 C-C-0.589600         0     1.91044   3.42352  -4.97504  H
 O-O--0.574800        0     1.32612   3.82824  -5.96688  H
 C-CT--0.007000       0     3.18783   1.45145  -5.74956  H
 C-CT-0.018900        0     2.31603   1.16603  -6.97538  H
 C-CT-0.019200        0     1.03613   0.57056  -6.37838  H
 H-H1-0.064100        0     2.47089   1.75974  -3.68029  H
 H-HC-0.025300        0     3.67824   0.54497  -5.38362  H
 H-HC-0.025300        0     3.95657   2.20651  -5.94127  H
 H-HC-0.021300        0     2.78111   0.4779   -7.68156  H
 H-HC-0.021300        0     2.08283   2.10181  -7.48491  H
 H-H1-0.039100        0     0.16284   0.84228  -6.9674   H
 H-H1-0.039100        0     1.10742  -0.51912  -6.34094  H
 N-N--0.415700        0     2.51648   4.19391  -4.03641  H
 C-CT-0.039700        0     2.83237   5.61884  -4.11446  H
 C-C-0.597300         0     3.94535   5.80458  -5.19896  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.01325   5.20097  -5.04375  L
 C-CT--0.003600       0     3.1292    6.0239   -2.63923  H
 C-CT-0.013600        0     4.22415   7.03831  -2.29406  H
 C-C-0.805400         0     4.77753   6.78755  -0.88882  H
 O-O2--0.818800       0     5.06432   5.66943  -0.4915   H
 H-H-0.271900         0     2.7415    3.74671  -3.16399  H
 H-H1-0.110500        0     1.9542    6.17125  -4.44777  H
 H-HC--0.017300       0     2.19195   6.35953  -2.18189  H
 H-HC--0.017300       0     3.36462   5.12459  -2.06034  H
 H-HC--0.042500       0     3.88626   8.06925  -2.39     H
 H-HC--0.042500       0     5.10095   6.94716  -2.95113  H
 N-N--0.254800        0     3.70515   6.50051  -6.34483  L
 C-CT--0.026600      -1     4.63889   6.634    -7.4896   L
 C-C-0.589600         0     6.06725   7.10313  -7.16901  L
 O-O--0.574800        0     6.96518   6.91941  -7.99226  L
 C-CT--0.007000       0     3.9531    7.48767  -8.55771  L
 C-CT-0.018900        0     2.62913   7.93668  -7.9472   L
 C-CT-0.019200        0     2.42076   7.09683  -6.69094  L
 H-H1-0.064100        0     4.74492   5.63623  -7.9083   L
 H-HC-0.025300        0     3.76276   6.87772  -9.44171  L
 H-HC-0.025300        0     4.55881   8.35135  -8.8334   L
 H-HC-0.021300        0     1.81368   7.78411  -8.65434  L
 H-HC-0.021300        0     2.68738   8.98784  -7.66767  L
 H-H1-0.039100        0     2.05612   7.73704  -5.88701  L
 H-H1-0.039100        0     1.69302   6.31072  -6.89456  L
 N-N--0.415700        0     6.32302   7.66316  -5.98697  L
 C-CT-0.014300       -1     7.66311   7.87343  -5.45422  L
 C-C-0.597300         0     8.4703    6.58225  -5.38626  L
 O-O--0.567900        0     8.25463   5.71337  -4.53893  L
 C-CT--0.204100       0     7.5743    8.5227   -4.05969  L
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C-C-0.713000          0     8.93605   8.9562   -3.53756  L
O-O--0.593100         0     9.5599    8.32717  -2.69338  L
N-N--0.919100         0     9.46915   10.04668  -4.03189  L
H-H-0.271900          0     5.51181   7.90381  -5.41522  L
H-H1-0.104800         0     8.17471   8.57155  -6.11857  L
H-HC-0.079700         0     7.1478    7.815    -3.35142  L
H-HC-0.079700         0     6.91756   9.38461  -4.10451  L
H-H-0.419600          0     10.35611   10.31451  -3.65391  L
H-H-0.419600          0     8.97943   10.6257  -4.71251  L
N-N--0.415700         0     9.4865    6.52049  -6.2328   L
C-CT--0.025200        -1    10.66864   5.74772  -5.93816  L
C-C-0.597300          0     11.02375   4.7351   -7.03109  L
O-O--0.567900         0     11.54247   5.08341  -8.0876   L
H-H-0.271900          0     9.50586   7.17987  -6.99704  L
H-H1-0.069800         0     10.57059   5.22707  -4.98492  L
H-H1-0.069800         0     11.50989   6.43409  -5.84597  L
N-N--0.415700         0     10.77294   3.46794  -6.72292  L
C-CT--0.001400        -1    10.8234   2.27364  -7.57734  L
C-C-0.597300          0     9.74539   1.33624  -6.99637  L
O-O--0.567900         0     8.8619    1.78509  -6.25444  L
C-CT--0.015200        0     12.2586   1.7029   -7.5768   L
C-CA--0.001100        0     12.7474   1.30088  -8.95439  L
C-CA--0.190600        0     13.13878   2.30558  -9.86125  L
C-CA--0.190600        0     12.81846  -0.05406  -9.33332  L
C-CA--0.234100        0     13.60471   1.96192  -11.14475  L
C-CA--0.234100        0     13.27498  -0.40165  -10.61951  L
C-C-0.322600          0     13.66983   0.60396  -11.52558  L
O-OH--0.557900        0     14.1064   0.26427  -12.76637  L
H-H-0.271900          0     10.25115   3.33853  -5.8673   L
H-H1-0.087600         0     10.534    2.54524  -8.59414  L
H-HC-0.029500         0     12.34054   0.86166  -6.88785  L
H-HC-0.029500         0     12.94909   2.46398  -7.20907  L
H-HA-0.169900         0     13.07144   3.34619  -9.56651  L
H-HA-0.169900         0     12.52482  -0.83391  -8.64579  L
H-HA-0.165600         0     13.89981   2.7384   -11.83268  L
H-HA-0.165600         0     13.32547  -1.43499  -10.92669  L
H-HO-0.399200         0     14.35013   1.03985  -13.27129  L
N-N--0.415700         0     9.87135   0.03324  -7.19615  L
C-CT--0.051800        -1    9.42137  -0.95219  -6.21446  L
C-C-0.597300          0     10.57696  -1.88662  -5.90412  L
O-O--0.567900         0     11.53438  -2.01503  -6.66745  L
C-CT--0.110200        0     8.13042  -1.63544  -6.71409  L
C-CT-0.353100         0     8.2185   -2.40722  -8.04868  L
C-CT--0.412100        0     8.7395   -3.83677  -7.86524  L
C-CT--0.412100        0     6.82154  -2.50361  -8.6625   L
H-H-0.271900          0     10.55197  -0.26666  -7.88142  L
H-H1-0.092200         0     9.18757  -0.42687  -5.29153  L
H-HC-0.045700         0     7.3872   -0.8435   -6.82142  L
H-HC-0.045700         0     7.75792  -2.31037  -5.94475  L
H-HC--0.036100        0     8.8608   -1.87939  -8.75244  L
H-HC-0.100000         0     9.77912  -3.82219  -7.54776  L
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 H-HC-0.100000        0     8.68701  -4.36611  -8.81664  L
 H-HC-0.100000        0     8.13929  -4.36656  -7.1264   L
 H-HC-0.100000        0     6.14199  -3.01673  -7.98713  L
 H-HC-0.100000        0     6.86618  -3.03268  -9.61536  L
 H-HC-0.100000        0     6.43949  -1.50347  -8.84635  L
 N-N--0.415700        0     10.51521  -2.49527  -4.73435  L
 C-CT--0.058100       -1    11.60665  -3.28172  -4.17642  L
 C-C-0.597300         0     11.11423  -4.67794  -3.81871  L
 O-O--0.567900        0     9.91888  -4.9617   -3.82161  L
 C-CT--0.007400       0     12.18679  -2.51972  -2.97091  L
 C-CC-0.186800        0     11.17122  -2.16832  -1.90564  L
 N-NB--0.543200       0     10.75253  -3.00162  -0.86799  L
 C-CW--0.220700       0     10.46538  -1.00314  -1.84639  L
 C-CR-0.163500        0     9.81062  -2.31352  -0.19978  L
 N-NA--0.279500       0     9.60659  -1.11835  -0.77495  L
 H-H-0.271900         0     9.67316  -2.3555   -4.18738  L
 H-H1-0.136000        0     12.39605  -3.402    -4.92036  L
 H-HC-0.036700        0     12.63383  -1.59291  -3.33324  L
 H-HC-0.036700        0     12.98554  -3.10676  -2.52299  L
 H-H4-0.186200        0     10.52935  -0.18233  -2.54776  L
 H-H-0.333900         0     8.86305  -0.47595  -0.5266   L
 H-H5-0.143500        0     9.25335  -2.68127   0.65273  L
 N-N--0.415700        0     12.03155  -5.58746  -3.5081   L
 C-CT--0.059700       -1    11.64384  -6.96308  -3.19407  L
 C-C-0.597300         0     10.72799  -7.09055  -1.95088  L
 O-O--0.567900        0     9.97417  -8.05521  -1.83719  L
 C-CT-0.130300        0     12.88209  -7.87043  -3.09439  L
 C-CT--0.043000       0     12.42815  -9.34226  -3.00207  L
 C-CT--0.320400       0     13.80736  -7.48068  -1.92607  L
 C-CT--0.066000       -1    13.49568  -10.31902  -3.47245  L
 H-H-0.271900         0     13.00749  -5.33771  -3.54023  L
 H-H1-0.086900        0     11.0612  -7.32188  -4.04013  L
 H-HC-0.018700        0     13.44261  -7.74744  -4.02328  L
 H-HC-0.023600        0     11.55685  -9.49652  -3.63943  L
 H-HC-0.023600        0     12.14986  -9.58756  -1.97619  L
 H-HC-0.088200        0     14.71241  -8.08405  -1.95981  L
 H-HC-0.088200        0     13.31138  -7.64519  -0.96875  L
 H-HC-0.088200        0     14.10408  -6.4355   -1.99913  L
 H-HC-0.018600        0     13.10432  -11.33515  -3.41569  L
 H-HC-0.018600        0     14.37949  -10.24824  -2.83886  L
 H-HC-0.018600        0     13.77057  -10.10362  -4.50559  L
 N-N--0.415700        0     10.73698  -6.11239  -1.03796  L
 C-CT--0.025200       -1    9.70958  -5.97871  -0.00356  L
 C-C-0.597300         0     8.31793  -5.8742   -0.62337  L
 O-O--0.567900        0     7.51273  -6.79803  -0.49488  L
 H-H-0.271900         0     11.34698  -5.32234  -1.18782  L
 H-H1-0.069800        0     9.90716  -5.09961   0.60512  L
 H-H1-0.069800        0     9.73116  -6.85722   0.63618  L
 N-N--0.415700        0     8.06343  -4.78863  -1.36475  L
 C-CT--0.058100       0     6.86642  -4.62135  -2.20372  L    H-HC
246   0.        0.
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C-C-0.597300         0     6.5233   -5.8926   -2.99501  L
O-O--0.567900        0     5.35421  -6.26448  -3.06156  L
C-CT--0.007400       0     7.04315  -3.46058  -3.18618  H
C-CC-0.186800        0     7.02703  -2.04422  -2.7075   H
N-NB--0.543200       0     7.66755  -1.11876  -3.49447  H
C-CW--0.220700       0     6.31624  -1.40651  -1.72365  H
C-CR-0.163500        0     7.29453   0.05351  -3.03374  H
N-NA--0.279500       0     6.49578  -0.05893  -1.94404  H
H-H-0.271900         0     8.82016  -4.12383  -1.47562  L
H-H1-0.136000        0     6.00677  -4.40609  -1.56594  L
H-HC-0.036700        0     6.24556  -3.56132  -3.93042  H
H-HC-0.036700        0     7.96291  -3.59912  -3.74847  H
H-H4-0.186200        0     5.67593  -1.75033  -0.93053  H
H-H-0.333900         0     5.94323   0.71013  -1.54631  H
H-H5-0.143500        0     7.57838   1.01939  -3.44276  H
N-N--0.415700        0     7.52107  -6.58205  -3.56253  L
C-CT-0.033700        -1    7.33751  -7.83857  -4.28931  L
C-C-0.597300         0     6.53692  -8.90859  -3.54232  L
O-O--0.567900        0     5.71401  -9.58273  -4.16127  L
C-CT--0.182500       0     8.65812  -8.3658   -4.85475  L
H-H-0.271900         0     8.44665  -6.17037  -3.5145   L
H-H1-0.082300        0     6.72653  -7.58699  -5.15439  L
H-HC-0.060300        0     9.20094  -7.55855  -5.34777  L
H-HC-0.060300        0     8.44602  -9.14253  -5.59072  L
H-HC-0.060300        0     9.26157  -8.80477  -4.06571  L
N-N--0.347900        0     6.70686  -9.05032  -2.22321  L
C-CT--0.240000       -1    5.82408  -9.91199  -1.42664  L
C-C-0.734100         0     4.34685  -9.46346  -1.48453  L
O-O--0.589400        0     3.47547  -10.31407  -1.64333  L
C-CT--0.009400       0     6.34223  -10.05017   0.01454  L
C-CT-0.018700        0     5.45725  -10.99446   0.85402  L
C-CT--0.047900       0     6.08486  -11.28796   2.22079  L
C-CT--0.014300       0     5.12695  -12.06318   3.13291  L
N-N3--0.385400       0     5.71517  -12.26229   4.48254  L
H-H-0.274700         0     7.38124  -8.43647  -1.77087  L
H-H1-0.142600        0     5.84123  -10.90495  -1.87946  L
H-HC-0.036200        0     6.37367  -9.06898   0.48711  L
H-HC-0.036200        0     7.3575   -10.44868  -0.02154  L
H-HC-0.010300        0     5.31587  -11.93534   0.31972  L
H-HC-0.010300        0     4.48372  -10.52825   1.00972  L
H-HC-0.062100        0     6.32676  -10.33709   2.69442  L
H-HC-0.062100        0     6.9978   -11.8672   2.07514  L
H-HP-0.113500        0     4.87409  -13.02227   2.67195  L
H-HP-0.113500        0     4.20593  -11.47746   3.2278   L
H-H-0.340000         0     4.99901  -12.52555   5.15564  L
H-H-0.340000         0     6.06696  -11.3697   4.82926  L
H-H-0.340000         0     6.46931  -12.93048   4.48277  L
N-N--0.415700        0     4.05399  -8.16345  -1.35481  L
C-CT--0.024900       -1    2.69925  -7.59554  -1.53377  L
C-C-0.597300         0     2.14888  -7.87037  -2.9438   L
O-O--0.567900        0     1.02612  -8.35883  -3.0427   L
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C-CT-0.211700        0     2.67105  -6.09189  -1.21514  L
O-OH--0.654600       0     1.32621  -5.66059  -1.13272  L
H-H-0.271900         0     4.83853  -7.52642  -1.30951  L
H-H1-0.084300        0     2.03176  -8.09075  -0.82772  L
H-H1-0.035200        0     3.19148  -5.52762  -1.98819  L
H-H1-0.035200        0     3.16063  -5.92176  -0.25702  L
H-HO-0.427500        0     1.2709   -4.73144  -0.83308  L
N-N--0.415700        0     2.92353  -7.63888  -4.02148  L
C-CT--0.059700       -1    2.59515  -8.06872  -5.40774  L
C-C-0.597300         0     2.18562  -9.55954  -5.38069  L
O-O--0.567900        0     1.06087  -9.88326  -5.74174  L
C-CT-0.130300        0     3.74548  -7.79061  -6.4067   L
C-CT--0.043000       0     4.1171   -6.29232  -6.42435  L
C-CT--0.320400       0     3.35122  -8.2442   -7.82509  L
C-CT--0.066000       0     5.348    -5.95485  -7.27182  L
H-H-0.271900         0     3.82213  -7.20061  -3.84616  L
H-H1-0.086900        0     1.72232  -7.50376  -5.73722  L
H-HC-0.018700        0     4.62102  -8.36041  -6.10172  L
H-HC-0.023600        0     4.32854  -5.9584   -5.41135  L
H-HC-0.023600        0     3.27121  -5.71717  -6.79774  L
H-HC-0.088200        0     2.51668  -7.64693  -8.19423  L
H-HC-0.088200        0     3.06756  -9.29669  -7.83709  L
H-HC-0.088200        0     4.19282  -8.12824  -8.50737  L
H-HC-0.018600        0     5.09902  -5.98829  -8.33252  L
H-HC-0.018600        0     6.15883  -6.6521   -7.06703  L
H-HC-0.018600        0     5.67754  -4.94992  -7.01832  L
N-N--0.415700        0     3.0518   -10.46583  -4.90831  L
C-CT-0.021300        -1    2.83477  -11.92553  -4.91525  L
C-C-0.597300         0     1.61536  -12.43435  -4.14767  L
O-O--0.567900        0     1.0715   -13.47588  -4.49994  L
C-CT--0.123100       -1    4.14702  -12.65812  -4.50105  L
S-SH--0.311900       0     5.49035  -12.31311  -5.67384  L
H-H-0.271900         0     3.95467  -10.1242  -4.6024   L
H-H1-0.112400        0     2.63763  -12.20887  -5.95111  L
H-H1-0.111200        0     3.95693  -13.73339  -4.49564  L
H-H1-0.111200        0     4.43866  -12.34716  -3.49709  L
H-HS-0.193300        0     5.6463   -11.01921  -5.35575  L
N-N--0.415700        0     1.18418  -11.72759  -3.10743  L
C-CT--0.051800       -1   -0.04787  -12.04107  -2.38979  L
C-C-0.597300         0    -1.28064  -11.40364  -3.05683  L
O-O--0.567900        0    -2.25319  -12.11238  -3.29066  L
C-CT--0.110200       0     0.09623  -11.56368  -0.93332  L
C-CT-0.353100        0     1.11785  -12.3838  -0.12138  L
C-CT--0.412100       0     1.46094  -11.65088   1.17349  L
C-CT--0.412100       0     0.58207  -13.76849   0.24979  L
H-H-0.271900         0     1.72082  -10.90871  -2.84918  L
H-H1-0.092200        0    -0.21484  -13.11894  -2.39583  L
H-HC-0.045700        0    -0.87494  -11.6258  -0.43988  L
H-HC-0.045700        0     0.39845  -10.51462  -0.94065  L
H-HC--0.036100       0     2.03978  -12.50707  -0.68878  L
H-HC-0.100000        0     1.90444  -10.68887   0.92067  L
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H-HC-0.100000        0     2.17205  -12.23331   1.75448  L
H-HC-0.100000        0     0.55525  -11.48266   1.75813  L
H-HC-0.100000        0     1.31745  -14.30512   0.84685  L
H-HC-0.100000        0     0.38791  -14.346    -0.65368  L
H-HC-0.100000        0    -0.34543  -13.67251   0.81521  L
N-N--0.415700        0    -1.25961  -10.10206  -3.38499  L
C-CT-0.014300       -1    -2.36226  -9.41422   -4.08561  L
C-C-0.597300         0    -2.71808  -10.10384  -5.38829  L
O-O--0.567900        0    -3.86521  -10.50395  -5.59     L
C-CT--0.204100       0    -2.09881  -7.90969   -4.19475  L
C-C-0.713000         0    -2.31508  -7.2251    -2.85312  L
O-O--0.593100        0    -3.42745  -6.92106   -2.44755  L
N-N--0.919100        0    -1.26985  -6.96234   -2.10917  L
H-H-0.271900         0    -0.40773  -9.58376   -3.20468  L
H-H1-0.104800        0    -3.2556   -9.53046   -3.4667   L
H-HC-0.079700        0    -2.81598  -7.48482   -4.8952   L
H-HC-0.079700        0    -1.096    -7.71577   -4.5727   L
H-H-0.419600         0    -1.40867  -6.45964   -1.25298  L
H-H-0.419600         0    -0.34575  -7.23326   -2.41737  L
N-N--0.415700        0    -1.70457  -10.33101  -6.21195  L
C-CT--0.002400      -1    -1.84204  -11.15613  -7.39062  L
C-C-0.597300         0    -2.01972  -12.65197  -7.14358  L
O-O--0.567900        0    -2.48755  -13.36688  -8.02432  L
C-CT--0.034300       0    -0.70806  -10.86569  -8.38966  L
C-CA-0.011800        0    -0.84745  -9.51776   -9.08122  L
C-CA--0.125600       0    -1.58106  -9.42199   -10.27969  L
C-CA--0.125600       0    -0.3016   -8.35056   -8.51213  L
C-CA--0.170400       0    -1.78269  -8.17148   -10.89152  L
C-CA--0.170400       0    -0.4933   -7.10097   -9.13049  L
C-CA--0.107200       0    -1.24243  -7.00968   -10.31556  L
H-H-0.271900         0    -0.78196  -9.99072   -5.96721  L
H-H1-0.097800        0    -2.76449  -10.85399  -7.88982  L
H-HC-0.029500        0    -0.72088  -11.63567  -9.16252  L
H-HC-0.029500        0     0.25881  -10.93582  -7.8941   L
H-HA-0.133000        0    -2.02173  -10.30582  -10.71848  L
H-HA-0.133000        0     0.24383  -8.4074   -7.58564  L
H-HA-0.143000        0    -2.3792   -8.09575  -11.79128  L
H-HA-0.143000        0    -0.08883  -6.20367  -8.68942  L
H-HA-0.129700        0    -1.4204   -6.04736  -10.77678  L
N-N--0.415700        0    -1.6896   -13.1184  -5.94548  L
C-CT--0.025200      -1    -1.89261  -14.49083  -5.51362  L
C-C-0.597300         0    -3.35058  -14.91219  -5.36649  L
O-O--0.567900        0    -3.69872  -16.05035  -5.66674  L
H-H-0.271900         0    -1.33706  -12.4636  -5.26618  L
H-H1-0.069800        0    -1.4029   -14.63487  -4.55139  L
H-H1-0.069800        0    -1.42179  -15.16054  -6.23373  L
N-N--0.415700        0    -4.19027  -14.00396  -4.87175  L
C-CT--0.059700      -1    -5.64952  -14.16771  -4.8071   L
C-C-0.597300         0    -6.3125   -14.13721  -6.18759  L
O-O--0.567900        0    -7.31651  -14.8167  -6.39507  L
C-CT-0.130300        0    -6.21233  -13.12025  -3.79001  L
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C-CT--0.043000       0    -5.88322  -13.60116  -2.33645  L
C-CT--0.320400       -1   -7.7294   -12.80531  -3.94323  L
C-CT--0.066000       -1   -5.2064   -12.58657  -1.38474  L
H-H-0.271900         0    -3.78295  -13.12063  -4.58868  L
H-H1-0.086900        0    -5.86843  -15.16212  -4.41606  L
H-HC-0.018700        0    -5.68341  -12.18199  -3.96566  L
H-HC-0.023600        0    -5.21783  -14.4643  -2.37951  L
H-HC-0.023600        0    -6.80139  -13.95129  -1.86303  L
H-HC-0.088200        0    -7.91803  -12.33404  -4.90995  L
H-HC-0.088200        0    -8.04594  -12.11771  -3.15896  L
H-HC-0.088200        0    -8.3108   -13.72567  -3.87837  L
H-HC-0.018600        0    -4.25533  -12.26238  -1.79788  L
H-HC-0.018600        0    -5.03625  -13.05157  -0.41359  L
H-HC-0.018600        0    -5.85466  -11.71904  -1.25956  L
N-N--0.415700        0    -5.72784  -13.39808  -7.1336   L
C-CT--0.149000       -1   -6.12473  -13.40583  -8.53021  L
H-H-0.271900         0    -4.90051  -12.88791  -6.86698  L
H-H1-0.097600        0    -6.39036  -14.41944  -8.83608  L
H-H1-0.097600        0    -5.30137  -13.04821  -9.14969  L
H-H1-0.097600        0    -6.99186  -12.75524  -8.66453  L
C-CT--0.366200       -1   -8.57567  -10.29048  -10.70464  L
C-C-0.597200         0    -7.82534  -9.60088  -9.6315   L
O-O--0.567900        0    -8.17218  -9.6253   -8.45834  L
H-HC-0.112300        0    -7.93364  -11.00747  -11.21063  L
H-HC-0.112300        0    -8.96865  -9.55129  -11.40103  L
H-HC-0.112300        0    -9.41554  -10.81316  -10.24529  L
N-N--0.415700        0    -6.77062  -8.97116  -10.09341  L
C-CT-0.021300        -1   -5.98371  -8.09009  -9.28947  L
C-C-0.597300         0    -5.49765  -6.93427  -10.16273  L
O-O--0.567900        0    -4.89595  -7.18755  -11.2102  L
C-CT--0.123100       0    -4.77704  -8.86559  -8.73901  L
S-SH--0.311900       0    -3.70627  -7.76197  -7.75971  L
H-H-0.271900         0    -6.591    -8.98498  -11.08443  L
H-H1-0.112400        0    -6.57481  -7.70311  -8.46057  L
H-H1-0.111200        0    -4.20615  -9.28048  -9.56902  L
H-H1-0.111200        0    -5.13288  -9.68864  -8.11899  L
H-HS-0.193300        0    -3.23821  -7.04383  -8.79379  L
N-N--0.415700        0    -5.72116  -5.68835  -9.74206  L
C-CT-0.014300        -1   -5.26874  -4.52276  -10.49688  L
C-C-0.597300         0    -3.90252  -3.9605   -10.01254  L
O-O--0.567900        0    -3.31145  -4.41939  -9.03027  L
C-CT--0.204100       0    -6.40559  -3.48575  -10.60358  L
C-C-0.713000         0    -6.22873  -2.51569  -11.77082  L
O-O--0.593100        0    -5.38504  -2.69666  -12.6392  L
N-N--0.919100        0    -6.96453  -1.44057  -11.82619  L
H-H-0.271900         0    -6.24715  -5.55557  -8.88307  L
H-H1-0.104800        0    -5.08503  -4.85653  -11.5198  L
H-HC-0.079700        0    -6.49943  -2.92549  -9.67375  L
H-HC-0.079700        0    -7.33641  -4.01952  -10.78201  L
H-H-0.419600         0    -6.84257  -0.83599  -12.60934  L
H-H-0.419600         0    -7.76236  -1.31385  -11.18762  L
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N-N--0.415700        0    -3.37052  -2.95633  -10.71003  L
C-CT--0.051800       -1   -2.21958  -2.1384   -10.32829  L
C-C-0.597300         0    -2.72045  -0.69003  -10.07181  L
O-O--0.567900        0    -3.14158  -0.02244  -11.01372  L
C-CT--0.110200       0    -1.15994  -2.19609  -11.44757  L
C-CT-0.353100        0     0.00979  -1.20477  -11.27147  L
C-CT--0.412100       0     0.82767  -1.49227  -10.01259  L
C-CT--0.412100       0     0.95655  -1.29053  -12.46932  L
H-H-0.271900         0    -3.90316  -2.64735  -11.52011  L
H-H1-0.092200        0    -1.78095  -2.51767  -9.40486  L
H-HC-0.045700        0    -1.65297  -1.96893  -12.39477  L
H-HC-0.045700        0    -0.76803  -3.21208  -11.50813  L
H-HC--0.036100       0    -0.36839  -0.18489  -11.21798  L
H-HC-0.100000        0     1.20159  -2.51505  -10.04401  L
H-HC-0.100000        0     0.20812  -1.35333  -9.12709  L
H-HC-0.100000        0     1.66374  -0.79613  -9.95214  L
H-HC-0.100000        0     1.38056  -2.292    -12.54237  L
H-HC-0.100000        0     1.75608  -0.55989  -12.35345  L
H-HC-0.100000        0     0.40404  -1.06456  -13.38159  L
N-N--0.347900        0    -2.67873  -0.19081  -8.82313  L
C-CT--0.263700       -1   -3.38469   1.03763  -8.37308  L
C-C-0.734100         0    -2.42533   2.07424  -7.80607  L
O-O--0.589400        0    -1.90919   1.90126  -6.71056  L
C-CT--0.000700       0    -4.43016   0.62604  -7.32773  L
C-CT-0.039000        0    -5.41472   1.7526   -6.9825   L
C-CT-0.048600        0    -6.08825   1.47925  -5.63518  L
N-N2--0.529500       0    -5.21853   1.85784  -4.5063   L
C-CA-0.807600        0    -5.5452    1.83642  -3.23284  L
N-N2--0.862700       0    -6.66407   1.35704  -2.80453  L
N-N2--0.862700       0    -4.74898   2.2955   -2.32313  L
H-H-0.274700         0    -2.23284  -0.75486  -8.10601  L
H-H1-0.156000        0    -3.91302   1.484    -9.21782  L
H-HC-0.032700        0    -3.90326   0.30855  -6.427    L
H-HC-0.032700        0    -5.00622  -0.22158  -7.70359  L
H-HC-0.028500        0    -6.17633   1.80395  -7.76204  L
H-HC-0.028500        0    -4.90596   2.71675  -6.93257  L
H-H1-0.068700        0    -6.39369   0.43629  -5.56925  L
H-H1-0.068700        0    -6.99869   2.05898  -5.57986  L
H-H-0.345600         0    -4.37771   2.4148   -4.68096  L
H-H-0.447800         0    -6.8753    1.39177  -1.81725  L
H-H-0.447800         0    -7.21255   0.71908  -3.38021  L
H-H-0.447800         0    -5.00967   2.2023   -1.35548  L
H-H-0.447800         0    -3.86815   2.72523  -2.62363  L
N-N--0.415700        0    -2.16916   3.13856  -8.55308  L
C-CT--0.002400       -1   -1.29716   4.2084   -8.07784  L
C-C-0.597300         0    -1.95583   5.03406  -6.9683   L
O-O--0.567900        0    -3.13686   5.36066  -7.04635  L
C-CT--0.034300       0    -0.84716   5.07656  -9.25821  L
C-CA-0.011800        0     0.12383   4.35038  -10.17331  L
C-CA--0.125600       0     1.50825   4.42991  -9.93012  L
C-CA--0.125600       0    -0.35087   3.5539   -11.23362  L
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 C-CA--0.170400       0     2.41212   3.73227  -10.75129  L
 C-CA--0.170400       0     0.55146   2.84039  -12.04296  L
 C-CA--0.107200       0     1.93399   2.93154  -11.80408  L
 H-H-0.271900         0    -2.67068   3.25671  -9.41577  L
 H-H1-0.097800        0    -0.40614   3.74866  -7.65381  L
 H-HC-0.029500        0    -0.35538   5.96975  -8.86884  L
 H-HC-0.029500        0    -1.71927   5.40594  -9.82572  L
 H-HA-0.133000        0     1.87296   5.02632  -9.1059   L
 H-HA-0.133000        0    -1.41278   3.47984  -11.42173  L
 H-HA-0.143000        0     3.47148   3.8132   -10.56555  L
 H-HA-0.143000        0     0.1732    2.22512  -12.84731  L
 H-HA-0.129700        0     2.62381   2.38776  -12.43137  L
 N-N--0.516300        0    -1.15773   5.371    -5.95549  L
 C-CT-0.038100        0    -1.56902   6.10859  -4.76019  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.79248   7.43391  -4.6654   L
 O-O--0.581900        0    -0.01488   7.65456  -3.73406  L
 C-CT--0.030300       0    -1.35156   5.21909  -3.52767  H
 C-C-0.799400         0    -2.27487   4.02185  -3.41258  H
 O-O2--0.801400       0    -2.07187   3.28059  -2.31358  H
 O-O2--0.801400       0    -3.18553   3.70624  -4.13836  H
 H-H-0.293600         0    -0.22182   4.98703  -5.98212  L
 H-H1-0.088000        0    -2.63127   6.35488  -4.82082  L
 H-HC--0.012200       0    -1.50875   5.80919  -2.61683  H
 H-HC--0.012200       0    -0.31322   4.86791  -3.50228  H
 N-N--0.516300        0    -0.99536   8.31551  -5.64661  L
 C-CT-0.038100        0    -0.31613   9.60868  -5.82585  L
 C-C-0.536600         0    -0.93892   10.74978  -4.99845  L
 O-O--0.581900        0    -0.87793   11.92309  -5.36588  L
 C-CT--0.030300       0    -0.27153   9.94718  -7.33079  L
 C-C-0.799400         0    -1.63379   10.22891  -7.97818  L
 O-O2--0.801400       0    -2.59458   9.49854  -7.64233  L
 O-O2--0.801400       0    -1.67397   11.09922  -8.87731  L
 H-H-0.293600         0    -1.72416   8.14067  -6.33833  L
 H-H1-0.088000        0     0.71087   9.50371  -5.48577  L
 H-HC--0.012200       0     0.17057   9.10689  -7.86037  L
 H-HC--0.012200       0     0.38511   10.80724  -7.47642  L
 N-N--0.415700        0    -1.50365   10.42213  -3.83166  L
 C-CT--0.038900      -1    -2.25068   11.35149  -2.96412  L
 C-C-0.597300         0    -1.36739   12.53722  -2.44215  L
 O-O--0.567900        0    -1.92642   13.5276  -1.97271  L
 C-CT-0.365400        0    -2.93581   10.64446  -1.80711  L
 O-OH--0.676100       0    -2.05743   9.81768  -1.06825  L
 C-CT--0.243800      -1    -4.04039   9.80816  -2.43245  L
 H-H-0.271900         0    -1.44264   9.45026  -3.56214  L
 H-H1-0.100700        0    -3.02411   11.82289  -3.57021  L
 H-H1-0.004300        0    -3.37823   11.37823  -1.13475  L
 H-HC-0.064200        0    -4.73216   10.45105  -2.97544  L
 H-HC-0.064200        0    -4.56769   9.31013  -1.62539  L
 H-HC-0.064200        0    -3.63232   9.05083  -3.10163  L
 H-HO-0.410200        0    -1.91499   10.29418  -0.21595  L
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 N-N--0.415700        0    -0.01676   12.5245  -2.57288  L
 C-CT-0.014300        -1    0.88666   13.70638  -2.44501  L
 C-C-0.597300         0     1.84113   13.81125  -3.66335  L
 O-O--0.567900        0     2.99079   13.37445  -3.56164  L
 C-CT--0.204100       0     1.61464   13.72699  -1.08914  L
 C-C-0.713000         0     2.36983   15.03766  -0.88192  L
 O-O--0.593100        0     2.67596   15.79983  -1.78879  L
 N-N--0.919100        0     2.70072   15.37489   0.3384   L
 H-H-0.271900         0     0.34295   11.71866  -3.06909  L
 H-H1-0.104800        0     0.25794   14.59522  -2.44656  L
 H-HC-0.079700        0     2.3188    12.8992  -1.03598  L
 H-HC-0.079700        0     0.8761    13.61603  -0.29363  L
 H-H-0.419600         0     3.17305   16.25491   0.40787  L
 H-H-0.419600         0     2.42139   14.82787   1.14142  L
 N-N--0.254800        0     1.43388   14.46453  -4.77745  L
 C-CT--0.026600       -1    2.18043   14.48048  -6.04711  L
 C-C-0.589600         0     3.54793   15.14953  -5.98753  L
 O-O--0.574800        0     4.37123   14.97396  -6.88305  L
 C-CT--0.007000       0     1.24219   15.10512  -7.08426  L
 C-CT-0.018900        0     0.28237   15.94422  -6.24609  L
 C-CT-0.019200        0     0.15719   15.14612  -4.95076  L
 H-H1-0.064100        0     2.353     13.44476  -6.34243  L
 H-HC-0.025300        0     0.68278   14.31155  -7.58379  L
 H-HC-0.025300        0     1.7747    15.71054  -7.81888  L
 H-HC-0.021300        0    -0.68303   16.06729  -6.73802  L
 H-HC-0.021300        0     0.73428   16.91429  -6.03434  L
 H-H1-0.039100        0    -0.05527   15.82451  -4.12454  L
 H-H1-0.039100        0    -0.64192   14.41024  -5.04655  L
 N-N--0.415700        0     3.84519   15.9032  -4.93151  L
 C-CT--0.025200       -1    5.01135   16.7743  -4.89844  L
 C-C-0.597300         0     6.3586    16.14044  -4.56324  L
 O-O--0.567900        0     7.29262   16.81588  -4.13617  L
 H-H-0.271900         0     3.19568   15.90685  -4.15322  L
 H-H1-0.069800        0     4.82985   17.55147  -4.15642  L
 H-H1-0.069800        0     5.11405   17.268   -5.8653   L
 N-N--0.347900        0     6.45352   14.84208  -4.80458  L
 C-CT--0.240000       -1    7.61916   13.96176  -4.70269  L
 C-C-0.734100         0     7.53329   12.88153  -5.81438  L
 O-O--0.589400        0     8.3141    11.92884  -5.78639  L
 C-CT--0.009400       0     7.60383   13.33866  -3.26905  L
 C-CT-0.018700        0     6.41913   12.36333  -3.12621  L    H-HC
590   0.        0.
 C-CT--0.047900       0     5.98258   11.73197  -1.79779  H
 C-CT--0.014300       0     4.77414   10.87904  -2.212    H
 N-N3--0.385400       0     4.09146   10.13017  -1.13845  H
 H-H-0.274700         0     5.5795    14.44224  -5.12622  L
 H-H1-0.142600        0     8.53436   14.53633  -4.84654  L
 H-HC-0.036200        0     7.51443   14.13311  -2.52608  L
 H-HC-0.036200        0     8.53526   12.80016  -3.09117  L
 H-HC-0.010300        0     6.6626    11.52869  -3.76661  L
 H-HC-0.010300        0     5.54098   12.87516  -3.50768  L
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H-HC-0.062100        0     5.69052   12.51822  -1.09841  H
H-HC-0.062100        0     6.78907   11.13326  -1.37518  H
H-HP-0.113500        0     5.07503   10.13331  -2.95775  H
H-HP-0.113500        0     4.04335   11.52486  -2.71936  H
H-H-0.340000         0     3.15826   9.92498  -1.50396  H
H-H-0.340000         0     3.9483    10.74028  -0.32765  H
H-H-0.340000         0     4.71206   8.70305  -0.52665  H
N-N--0.516300        0     6.55641   12.96541  -6.73508  L
C-CT-0.039700        -1    6.06988   11.85605  -7.58188  L
C-C-0.536600         0     6.24522   12.16984  -9.09639  L
O-O--0.581900        0     6.04622   13.30225  -9.52749  L
C-CT-0.056000        0     4.65585   11.36522  -7.18298  L
C-CT-0.013600        0     4.6349    11.156   -5.66315  L
C-C-0.805400         0     3.69081   10.11928  -5.04888  L
O-O2--0.818800       0     2.65001   10.4971  -4.47702  L
O-O2--0.818800       0     4.16286   8.96821  -4.91461  L
H-H-0.293600         0     5.99949   13.81125  -6.80021  L
H-H1-0.110500        0     6.72559   11.00524  -7.39785  L
H-HC--0.017300       0     4.46866   10.4203  -7.6878   L
H-HC--0.017300       0     3.89758   12.09139  -7.47473  L
H-HC--0.042500       0     4.46498   12.12612  -5.20533  L
H-HC--0.042500       0     5.63132   10.81384  -5.39699  L
N-N--0.415700        0     6.70816   11.19396  -9.90611  L
C-CT--0.149000       -1    7.10696   11.36961  -11.32136  L
H-H-0.271900         0     6.83024   10.28359  -9.49071  L
H-H1-0.097600        0     7.89592   12.12061  -11.38798  L
H-H1-0.097600        0     6.24708   11.71798  -11.8973  L
H-H1-0.097600        0     7.46198   10.4253  -11.73484  L
C-CT--0.366200       0     10.21565   1.7334   -12.22223  L
C-C-0.597200         0     9.1202    1.10343  -11.39576  L
O-O--0.567900        0     9.37708   0.68821  -10.27128  L
H-HC-0.112300        0     10.76208   2.4292   -11.58805  L
H-HC-0.112300        0     9.80319   2.26642  -13.07591  L
H-HC-0.112300        0     10.8895   0.94714  -12.55726  L
N-N--0.415700        0     7.90526   1.04859  -11.95098  L
C-CT--0.059700       -1    6.72269   0.43508  -11.32129  L
C-C-0.597300         0     5.96788  -0.46039  -12.32185  L
O-O--0.567900        0     6.16925  -1.67069  -12.3133  L
C-CT-0.130300        0     5.83527   1.48215  -10.58732  L
C-CT--0.043000       0     6.63441   2.18144  -9.45578  L
C-CT--0.320400       0     4.57484   0.82128  -9.98982  L
C-CT--0.066000       0     5.8878    3.28949  -8.70414  L
H-H-0.271900         0     7.8241    1.40252  -12.88922  L
H-H1-0.086900        0     7.0856   -0.24989  -10.55549  L
H-HC-0.018700        0     5.51879   2.23809  -11.30795  L
H-HC-0.023600        0     7.51786   2.65364  -9.8822   L
H-HC-0.023600        0     6.96834   1.43449  -8.73351  L
H-HC-0.088200        0     3.99768   0.29417  -10.74759  L
H-HC-0.088200        0     3.9167    1.57821  -9.56626  L
H-HC-0.088200        0     4.8521    0.11907  -9.20482  L
H-HC-0.018600        0     5.05584   2.8803   -8.13232  L
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H-HC-0.018600        0     5.52257   4.03185  -9.41322  L
H-HC-0.018600        0     6.57439   3.7759   -8.01021  L
N-N--0.415700        0     5.11211   0.107    -13.18544  L
C-CT--0.149000       -1    4.2842   -0.64702  -14.1333  L
H-H-0.271900         0     4.98998   1.10495  -13.12271  L
H-H1-0.097600        0     3.80965  -1.48798  -13.62241  L
H-H1-0.097600        0     4.90786  -1.03946  -14.9383  L
H-H1-0.097600        0     3.50907  -0.00524  -14.55499  L
C-CT--0.366200       -1   -5.13068   16.91483  -3.20718  L
C-C-0.597200         0    -5.70318   16.1517  -2.02603  L
O-O--0.567900        0    -5.55055   16.60796  -0.89589  L
H-HC-0.112300        0    -5.93992   17.30544  -3.81904  L
H-HC-0.112300        0    -4.49551   16.24742  -3.78855  L
H-HC-0.112300        0    -4.5262    17.73763  -2.83003  L
N-N--0.254800        0    -6.4211    15.04258  -2.26652  L
C-CT--0.026600       -1   -7.10071   14.28834  -1.21955  L
C-C-0.589600         0    -6.23403   13.1972  -0.59466  L
O-O--0.574800        0    -5.6996    12.31791  -1.26744  L
C-CT--0.007000       0    -8.30051   13.66582  -1.9435   L
C-CT-0.018900        0    -7.7665    13.38519  -3.35096  L
C-CT-0.019200        0    -6.7816    14.53177  -3.58525  L
H-H1-0.064100        0    -7.46368   14.96073  -0.44163  L
H-HC-0.025300        0    -9.10732   14.39781  -2.00206  L
H-HC-0.025300        0    -8.65345   12.75735  -1.4559   L
H-HC-0.021300        0    -8.56697   13.38516  -4.09112  L
H-HC-0.021300        0    -7.23531   12.43337  -3.37281  L
H-H1-0.039100        0    -5.9006    14.16627  -4.11539  L
H-H1-0.039100        0    -7.27127   15.31606  -4.1632   L
N-N--0.415700        0    -6.16871   13.24436   0.72855  L
C-CT--0.023700       -1   -5.31597   12.40981   1.56204  L
C-C-0.597300         0    -5.5085    10.88308   1.42854  L
O-O--0.567900        0    -6.5983    10.39834   1.11162  L
C-CT-0.034200        0    -5.56552   12.77664   3.03881  L
C-CT-0.001800        0    -5.15035   14.20258   3.43207  L
S-S--0.273700        0    -3.37107   14.49915   3.63996  L
C-CT--0.053600       -1   -3.03796   13.52444   5.13606  L
H-H-0.271900         0    -6.64881   14.0076   1.17183  L
H-H1-0.088000        0    -4.27345   12.62991   1.31891  L
H-HC-0.024100        0    -5.03673   12.07389   3.68243  L
H-HC-0.024100        0    -6.63088   12.66052   3.24475  L
H-H1-0.044000        0    -5.63417   14.44272   4.37891  L
H-H1-0.044000        0    -5.52866   14.90289   2.68762  L
H-H1-0.068400        0    -3.19678   12.46548   4.93006  L
H-H1-0.068400        0    -3.69552   13.84361   5.94381  L
H-H1-0.068400        0    -1.99922   13.66314   5.43394  L
N-N--0.415700        0    -4.44828   10.1382   1.767    L
C-CT--0.001400       -1   -4.29778   8.68544   1.63682  L
C-C-0.597300         0    -5.52187   7.79696   1.95518  L
O-O--0.567900        0    -6.11787   7.28889   1.01055  L
C-CT--0.015200       0    -3.00549   8.20252   2.31495  L
C-CA--0.001100       0    -2.88496   6.69754   2.46778  L
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C-CA--0.190600       0    -2.87196   5.8563    1.33571  L
C-CA--0.190600       0    -2.898     6.13841   3.75784  L
C-CA--0.234100       0    -2.92428   4.45626   1.49982  L
C-CA--0.234100       0    -2.95462   4.74603   3.92244  L
C-C-0.322600         0    -2.98642   3.90125   2.79805  L
O-OH--0.557900       0    -3.10661   2.56017   2.97242  L
H-H-0.271900         0    -3.58495   10.64471   1.94484  L
H-H1-0.087600        0    -4.12953   8.51733   0.57293  L
H-HC-0.029500        0    -2.94266   8.66104   3.29913  L
H-HC-0.029500        0    -2.1579    8.5442    1.72551  L
H-HA-0.169900        0    -2.8956    6.2943    0.34546  L
H-HA-0.169900        0    -2.93886   6.77259   4.63511  L
H-HA-0.165600        0    -3.00328   3.80742   0.64148  L
H-HA-0.165600        0    -3.03862   4.33775   4.91821  L
H-HO-0.399200        0    -3.48696   2.38572   3.85467  L
N-N--0.516300        0    -5.87262   7.51119   3.21823  L
C-CT-0.038100        -1   -6.83283   6.43694   3.58083  L
C-C-0.536600         0    -8.23754   6.66447   3.01423  L
O-O--0.581900        0    -8.90681   5.70844   2.62878  L
C-CT--0.030300       0    -6.88629   6.22264   5.10665  L
C-C-0.799400         0    -5.84227   5.20981   5.59659  L
O-O2--0.801400       0    -5.9822    4.00581   5.27402  L
O-O2--0.801400       0    -4.89725   5.62007   6.30613  L
H-H-0.293600         0    -5.39358   8.01506   3.95835  L
H-H1-0.088000        0    -6.47221   5.5051    3.15039  L
H-HC--0.012200       0    -7.86894   5.83201   5.37505  L
H-HC--0.012200       0    -6.76599   7.17691   5.62182  L
N-N--0.415700        0    -8.67133   7.9242    2.92157  L
C-CT--0.002400       0    -9.86642   8.31951   2.17382  L
C-C-0.597300         0    -9.78218   7.86268   0.70832  L
O-O--0.567900        0    -10.64789   7.13061   0.22799  L
C-CT--0.034300       0    -10.06029   9.83941   2.28749  L
C-CA-0.011800        0    -11.1184   10.38934   1.34916  L
C-CA--0.125600       0    -12.48423   10.2469   1.65743  L
C-CA--0.125600       0    -10.73567   10.99003   0.13433  L
C-CA--0.170400       0    -13.46209   10.70786   0.75705  L
C-CA--0.170400       0    -11.71239   11.44822  -0.76681  L
C-CA--0.107200       0    -13.07629   11.30799  -0.45514  L
H-H-0.271900         0    -8.01461   8.63333   3.21534  L
H-H1-0.097800        0    -10.73458   7.82564   2.61165  L
H-HC-0.029500        0    -9.11407   10.33835   2.07369  L
H-HC-0.029500        0    -10.33327   10.08406   3.31471  L
H-HA-0.133000        0    -12.78231   9.76408   2.57704  L
H-HA-0.133000        0    -9.68764   11.0718  -0.12226  L
H-HA-0.143000        0    -14.50968   10.5834   0.98976  L
H-HA-0.143000        0    -11.40867   11.88785  -1.70627  L
H-HA-0.129700        0    -13.82671   11.64725  -1.1546   L
N-N--0.415700        0    -8.74515   8.28724  -0.01122  L
C-CT--0.038900       -1   -8.56521   7.96978  -1.43265  L
C-C-0.597300         0    -8.40471   6.48587  -1.70475  L
O-O--0.567900        0    -9.06803   5.92682  -2.57597  L
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C-CT-0.365400        0    -7.40825   8.7853   -2.02062  L
O-OH--0.676100       0    -7.66341   10.15912  -1.81318  L
C-CT--0.243800       0    -7.25836   8.58867  -3.52984  L
H-H-0.271900         0    -8.0558    8.88891   0.42957  L
H-H1-0.100700        0    -9.46899   8.28308  -1.95472  L
H-H1-0.004300        0    -6.48973   8.50019  -1.51363  L
H-HC-0.064200        0    -8.20565   8.79865  -4.02662  L
H-HC-0.064200        0    -6.95225   7.566    -3.74908  L
H-HC-0.064200        0    -6.50091   9.26606  -3.92114  L
H-HO-0.410200        0    -6.82298   10.60148  -1.6146   L
N-N--0.415700        0    -7.55032   5.84606  -0.9182   L
C-CT--0.058100       -1   -7.39275   4.40618  -0.79566  L
C-C-0.597300         0    -8.72669   3.69137  -0.64174  L
O-O--0.567900        0    -9.02736   2.81582  -1.45267  L
C-CT--0.007400       0    -6.42108   4.17403   0.36775  L
C-CC-0.186800        0    -6.3077    2.7597    0.84452  L
N-NB--0.543200       0    -6.3531    1.62873   0.03832  L
C-CW--0.220700       0    -6.23807   2.3811    2.14764  L
C-CR-0.163500        0    -6.35492   0.58037   0.86903  L
N-NA--0.279500       0    -6.26413   1.00829   2.13801  L
H-H-0.271900         0    -7.07165   6.42377  -0.23333  L
H-H1-0.136000        0    -6.93962   4.02233  -1.70946  L
H-HC-0.036700        0    -6.76111   4.76498   1.21131  L
H-HC-0.036700        0    -5.432     4.53031   0.08116  L
H-H4-0.186200        0    -6.22032   3.03306   3.01217  L
H-H-0.333900         0    -6.27486   0.4031    2.95677  L
H-H5-0.143500        0    -6.44494  -0.4531    0.55769  L
N-N--0.415700        0    -9.53543   4.07562   0.35125  L
C-CT-0.021300        -1   -10.83268   3.4474    0.55617  L
C-C-0.597300         0    -11.7449   3.48779  -0.64733  L
O-O--0.567900        0    -12.36247   2.48541  -1.00417  L
C-CT--0.123100       0    -11.48925   3.84343   1.89594  L
S-SH--0.311900       0    -12.57391   5.2972    1.81333  L
H-H-0.271900         0    -9.23632   4.80356   0.99273  L
H-H1-0.112400        0    -10.60894   2.38494   0.66522  L
H-H1-0.111200        0    -10.71706   4.00983   2.64692  L
H-H1-0.111200        0    -12.09263   3.00087   2.23711  L
H-HS-0.193300        0    -11.6554   6.13779   1.31669  L
N-N--0.415700        0    -11.78601   4.64587  -1.28518  L
C-CT--0.059700       -1   -12.61536   4.86197  -2.44322  L
C-C-0.597300         0    -12.14573   4.1351   -3.70435  L
O-O--0.567900        0    -12.96235   3.51168  -4.3791   L
C-CT-0.130300        0    -12.85138   6.38557  -2.62696  L
C-CT--0.043000       0    -14.18845   6.82652  -1.98029  L
C-CT--0.320400       -1   -12.76376   6.88771  -4.07291  L
C-CT--0.066000       -1   -15.47737   6.41445  -2.72284  L
H-H-0.271900         0    -11.24014   5.41064  -0.90308  L
H-H1-0.086900        0    -13.58248   4.41248  -2.22031  L
H-HC-0.018700        0    -12.06     6.91431  -2.09176  L
H-HC-0.023600        0    -14.18472   7.91409  -1.89522  L
H-HC-0.023600        0    -14.23003   6.4265   -0.96593  L
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H-HC-0.088200        0    -11.74517   6.7749   -4.44592  L
H-HC-0.088200        0    -13.01613   7.94745  -4.11003  L
H-HC-0.088200        0    -13.44669   6.33377  -4.71853  L
H-HC-0.018600        0    -16.34263   6.71931  -2.13401  L
H-HC-0.018600        0    -15.50943   5.33376  -2.86082  L
H-HC-0.018600        0    -15.52856   6.90514  -3.69458  L
N-N--0.415700        0    -10.8583   4.22045  -4.03455  L
C-CT--0.024900       -1   -10.25107   3.51829  -5.17055  L
C-C-0.597300         0    -10.4634   1.99616  -5.00723  L
O-O--0.567900        0    -10.93848   1.35324  -5.93729  L
C-CT-0.211700        0    -8.79306   3.96768  -5.2743   L
O-OH--0.654600       0    -8.30428   3.78978  -6.58712  L
H-H-0.271900         0    -10.26098   4.76317  -3.41881  L
H-H1-0.084300        0    -10.76633   3.82611  -6.08076  L
H-H1-0.035200        0    -8.18364   3.43568  -4.54343  L
H-H1-0.035200        0    -8.73943   5.03413  -5.05013  L
H-HO-0.427500        0    -7.51805   4.33363  -6.70015  L
N-N--0.516300        0    -10.24163   1.42295  -3.80989  L
C-CT-0.038100        -1   -10.54429   0.00523  -3.51068  L
C-C-0.536600         0    -12.02463  -0.38473  -3.64344  L
O-O--0.581900        0    -12.35508  -1.34405  -4.34725  L
C-CT--0.030300       0    -9.9928   -0.42553  -2.13471  L
C-C-0.799400         0    -8.57125  -0.97965  -2.22691  L
O-O2--0.801400       0    -7.96352  -0.90212  -3.31607  L
O-O2--0.801400       0    -8.03663  -1.48485  -1.21443  L
H-H-0.293600         0    -9.8883    2.00394  -3.05673  L
H-H1-0.088000        0    -10.05386  -0.58445  -4.28207  L
H-HC--0.012200       0    -10.62481  -1.21441  -1.72462  L
H-HC--0.012200       0    -10.02653   0.40979  -1.43551  L
N-N--0.415700        0    -12.9149   0.33668  -2.95901  L
C-CT-0.033700        -1   -14.36749   0.18659  -3.0616   L
C-C-0.597300         0    -14.85365   0.1955   -4.52316  L
O-O--0.567900        0    -15.69009  -0.61998  -4.90808  L
C-CT--0.182500       -1   -14.98374   1.34621  -2.33904  L
H-H-0.271900         0    -12.56216   1.10019  -2.39059  L
H-H1-0.082300        0    -14.67631  -0.75143  -2.59968  L
H-HC-0.060300        0    -14.71114   1.3093   -1.2839   L
H-HC-0.060300        0    -16.07034   1.2868   -2.41414  L
H-HC-0.060300        0    -14.65023   2.29326  -2.76218  L
N-N--0.415700        0    -14.36272   1.16286  -5.30444  L
C-CT--0.025200       -1   -14.73098   1.41063  -6.69348  L
C-C-0.597300         0    -14.23724   0.34397  -7.66687  L
O-O--0.567900        0    -14.98192  -0.07712  -8.54752  L
H-H-0.271900         0    -13.69082   1.79692  -4.88312  L
H-H1-0.069800        0    -14.31582   2.36865  -7.0041   L
H-H1-0.069800        0    -15.81672   1.46191  -6.77112  L
N-N--0.516300        0    -12.98072  -0.06893  -7.51606  L
C-CT-0.039700        -1   -12.34327  -1.15985  -8.25756  L
C-C-0.536600         0    -13.06861  -2.50702  -8.0793   L
O-O--0.581900        0    -13.20518  -3.26939  -9.03337  L
C-CT-0.056000        0    -10.87531  -1.21286  -7.80223  L
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C-CT-0.013600        0    -9.9989   -2.30119  -8.43307  L
C-C-0.805400         0    -9.56709  -2.01894  -9.8747   L
O-O2--0.818800       0    -9.56052  -2.9676   -10.69133  L
O-O2--0.818800       0    -9.07418  -0.90283  -10.14458  L
H-H-0.293600         0    -12.41267   0.38889  -6.80822  L
H-H1-0.110500        0    -12.36241  -0.92576  -9.32274  L
H-HC--0.017300       0    -10.87679  -1.3708   -6.72613  L
H-HC--0.017300       0    -10.41085  -0.24366  -7.98502  L
H-HC--0.042500       0    -10.52179  -3.25156  -8.36934  L
H-HC--0.042500       0    -9.08971  -2.3896   -7.83548  L
N-N--0.415700        0    -13.52063  -2.81019  -6.85763  L
C-CT--0.025200       -1   -14.21866  -4.05619  -6.50481  L
C-C-0.597300         0    -13.46927  -4.90871  -5.49631  L
O-O--0.567900        0    -13.807   -6.08388  -5.33343  L
H-H-0.271900         0    -13.39689  -2.09438  -6.15022  L
H-H1-0.069800        0    -14.3873  -4.6601   -7.39678  L
H-H1-0.069800        0    -15.18868  -3.80353  -6.07857  L
N-N--0.415700        0    -12.46126  -4.34262  -4.81602  L
C-CT--0.059700       -1   -11.72283  -5.04283  -3.76454  L
C-C-0.597300         0    -12.73762  -5.58379  -2.7526   L
O-O--0.567900        0    -13.67032  -4.88758  -2.3574   L
C-CT-0.130300        0    -10.64985  -4.14293  -3.0969   L
C-CT--0.043000       0    -9.34062  -4.12415  -3.90397  L
C-CT--0.320400       0    -10.22932  -4.62565  -1.69173  L
C-CT--0.066000       0    -9.41353  -3.50684  -5.29454  L
H-H-0.271900         0    -12.30783  -3.34858  -4.94948  L
H-H1-0.086900        0    -11.2275  -5.88873  -4.22327  L
H-HC-0.018700        0    -11.03729  -3.13112  -2.99919  L
H-HC-0.023600        0    -9.00274  -5.1448   -4.00909  L
H-HC-0.023600        0    -8.58652  -3.57792  -3.34126  L
H-HC-0.088200        0    -9.47009  -3.95645  -1.28239  L
H-HC-0.088200        0    -9.82674  -5.63806  -1.74059  L
H-HC-0.088200        0    -11.07533  -4.59883  -1.01294  L
H-HC-0.018600        0    -8.42261  -3.51787  -5.74595  L
H-HC-0.018600        0    -9.75057  -2.47962  -5.21148  L
H-HC-0.018600        0    -10.09271  -4.07134  -5.92909  L
N-N--0.415700        0    -12.54971  -6.83469  -2.32957  L
C-CT--0.025200       -1   -13.40358  -7.48169  -1.32529  L
C-C-0.597300         0    -12.85212  -7.41288   0.08189  L
O-O--0.567900        0    -13.58237  -7.21748   1.0514   L
H-H-0.271900         0    -11.80328  -7.33888  -2.79089  L
H-H1-0.069800        0    -13.53006  -8.53017  -1.59024  L
H-H1-0.069800        0    -14.392   -7.01953  -1.32591  L
N-N--0.415700        0    -11.5423  -7.5955    0.17536  L
C-CT--0.058100       -1   -10.78889  -7.58122   1.41067  L
C-C-0.597300         0    -9.41425  -6.93289   1.14144  L
O-O--0.567900        0    -8.67419  -7.42099   0.28814  L
C-CT--0.007400       0    -10.63328  -9.02329   1.92438  L
C-CC-0.186800        0    -11.92747  -9.61753   2.43225  L
N-NB--0.543200       0    -12.52709  -9.34395   3.66484  L
C-CW--0.220700       0    -12.74216  -10.44733   1.71886  L
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C-CR-0.163500        0    -13.69547  -10.00011   3.65845  L
N-NA--0.279500       0    -13.85056  -10.67566   2.50584  L
H-H-0.271900         0    -11.01984  -7.70692  -0.68179  L
H-H1-0.136000        0    -11.31131  -6.99397   2.16755  L
H-HC-0.036700        0    -9.89751  -9.04353   2.72587  L
H-HC-0.036700        0    -10.24477  -9.65118   1.12109  L
H-H4-0.186200        0    -12.5574  -10.80254   0.7153   L
H-H-0.333900         0    -14.66706  -11.21194   2.253    L
H-H5-0.143500        0    -14.41513  -9.97477   4.46657  L
N-N--0.415700        0    -9.07171  -5.82379   1.80972  L
C-CT--0.024900       -1   -7.81298  -5.08747   1.57616  L
C-C-0.597300         0    -6.61972  -5.71199   2.30014  L
O-O--0.567900        0    -6.6678   -6.00155   3.49558  L
C-CT-0.211700        0    -7.94416  -3.59329   1.89826  L
O-OH--0.654600       0    -6.66698  -2.96804   1.86233  L
H-H-0.271900         0    -9.68894  -5.52581   2.55718  L
H-H1-0.084300        0    -7.6012   -5.13838   0.50741  L
H-H1-0.035200        0    -8.38687  -3.47337   2.88038  L
H-H1-0.035200        0    -8.60089  -3.12026   1.16566  L
H-HO-0.427500        0    -6.68867  -2.1924    2.45569  L
N-N--0.415700        0    -5.5208   -5.88728   1.56372  L
C-CT--0.051800       -1   -4.22166  -6.29777   2.09045  L
C-C-0.597300         0    -3.32228  -5.09379   2.30496  L
O-O--0.567900        0    -3.06562  -4.3476    1.36202  L
C-CT--0.110200       0    -3.55581  -7.30029   1.12315  L
C-CT-0.353100        0    -4.06698  -8.75266   1.18155  L
C-CT--0.412100       0    -5.46957  -8.93581   0.60126  L
C-CT--0.412100       0    -3.11616  -9.64451   0.37626  L
H-H-0.271900         0    -5.59662  -5.6624    0.58352  L
H-H1-0.092200        0    -4.35869  -6.79291   3.05495  L
H-HC-0.045700        0    -2.49614  -7.32859   1.36678  L
H-HC-0.045700        0    -3.63886  -6.93244   0.10348  L
H-HC--0.036100       0    -4.06125  -9.09343   2.21718  L
H-HC-0.100000        0    -5.51785  -8.53343  -0.41123  L
H-HC-0.100000        0    -6.20342  -8.42786   1.22488  L
H-HC-0.100000        0    -5.73017  -9.993     0.57969  L
H-HC-0.100000        0    -2.10783  -9.57324   0.78307  L
H-HC-0.100000        0    -3.10952  -9.33142  -0.66854  L
H-HC-0.100000        0    -3.4461   -10.6814   0.43549  L
N-N--0.415700        0    -2.8035   -4.9467    3.51668  L
C-CT-0.021300        -1   -1.86245  -3.88674   3.84717  L
C-C-0.597300         0    -0.72742  -4.3954    4.75384  L
O-O--0.567900        0    -0.7213   -5.55693   5.16472  L
C-CT--0.123100       0    -2.66983  -2.73974   4.46578  L
S-SH--0.311900       0    -1.72587  -1.19338   4.461    L
H-H-0.271900         0    -3.08288  -5.58611   4.25309  L
H-H1-0.112400        0    -1.39464  -3.51217   2.93309  L
H-H1-0.111200        0    -2.96712  -2.99478   5.48461  L
H-H1-0.111200        0    -3.56786  -2.58041   3.86793  L
H-HS-0.193300        0    -2.66014  -0.45271   5.07576  L
N-N--0.415700        0     0.25032  -3.55211   5.0836   L
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C-CT--0.038900       -1    1.37095  -3.91628   5.96288  L
C-C-0.597300         0     1.5016   -3.01044   7.16363  L
O-O--0.567900        0     0.85353  -1.97769   7.30569  L
C-CT-0.365400        0     2.71677  -4.03125   5.22216  L
O-OH--0.676100       0     3.08225  -2.83864   4.56382  L
C-CT--0.243800       0     2.71681  -5.18719   4.22544  L
H-H-0.271900         0     0.14722  -2.59118   4.77842  L
H-H1-0.100700        0     1.17032  -4.90377   6.37868  L
H-H1-0.004300        0     3.49939  -4.25562   5.94692  L
H-HC-0.064200        0     1.98356  -5.01794   3.43882  L
H-HC-0.064200        0     2.46588  -6.11602   4.73865  L
H-HC-0.064200        0     3.70489  -5.28181   3.78454  L
H-HO-0.410200        0     3.39556  -2.20092   5.24642  L
N-N--0.415700        0     2.33247  -3.49579   8.07694  L
C-CT--0.051800       -1    2.24909  -3.18789   9.48244  L
C-C-0.597300         0     2.3436   -1.6881    9.86063  L
O-O--0.567900        0     1.82024  -1.30298   10.8969  L
C-CT--0.110200       0     3.25272  -4.05821   10.20799  L
C-CT-0.353100        0     2.95333  -4.13281   11.70685  L
C-CT--0.412100       0     1.62105  -4.79855   12.06228  L
C-CT--0.412100       -1    4.06102  -5.00671   12.23213  L
H-H-0.271900         0     2.76826  -4.36873   7.83864  L
H-H1-0.092200        0     1.24659  -3.49069   9.78624  L
H-HC-0.045700        0     4.24968  -3.64561   10.04501  L
H-HC-0.045700        0     3.21315  -5.06792   9.79411  L
H-HC--0.036100       0     3.02873  -3.15485   12.17791  L
H-HC-0.100000        0     1.51777  -5.7591    11.55911  L
H-HC-0.100000        0     0.79182  -4.15183   11.7817  L
H-HC-0.100000        0     1.55683  -4.94321   13.14172  L
H-HC-0.100000        0     3.95194  -5.09776   13.31366  L
H-HC-0.100000        0     5.03077  -4.55245   12.03164  L
H-HC-0.100000        0     4.01164  -6.00324   11.79353  L
N-N--0.516300        0     2.98829  -0.83817   9.05659  L
C-CT-0.039700        -1    3.11134   0.61497   9.30462  L
C-C-0.536600         0     1.83293   1.44383   9.06745  L
O-O--0.581900        0     1.86428   2.66218   9.23368  L
C-CT-0.056000        0     4.31443   1.15342   8.49255  L
C-CT-0.013600        0     4.22594   1.06986   6.95291  L
C-C-0.805400         0     4.79717  -0.22153   6.34558  L
O-O2--0.818800       0     4.1837   -1.30907   6.47211  L
O-O2--0.818800       0     5.91236  -0.19763   5.76127  L
H-H-0.293600         0     3.29152  -1.1918    8.15324  L
H-H1-0.110500        0     3.34446   0.75918   10.3603  L
H-HC--0.017300       0     5.21889   0.6355    8.81663  L
H-HC--0.017300       0     4.44868   2.20226   8.7596   L
H-HC--0.042500       0     4.80957   1.89794   6.55098  L
H-HC--0.042500       0     3.19518   1.20981   6.6363   L
N-N--0.415700        0     0.71856   0.79355   8.72154  L
C-CT--0.002400       -1   -0.60268   1.40745   8.53948  L
C-C-0.597300         0    -1.72663   0.77396   9.37175  L
O-O--0.567900        0    -2.90036   1.12261   9.23676  L
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C-CT--0.034300       0    -1.00559   1.25225   7.06054  L
C-CA-0.011800        0    -0.10653   1.84526   5.99046  L
C-CA--0.125600       0    -0.32661   3.1617    5.54916  L
C-CA--0.125600       0     0.84939   1.04486   5.33451  L
C-CA--0.170400       0     0.37983   3.66391   4.44361  L
C-CA--0.170400       0     1.58901   1.56026   4.25381  L
C-CA--0.107200       0     1.34854   2.86982   3.80491  L
H-H-0.271900         0     0.80698  -0.19351   8.51516  L
H-H1-0.097800        0    -0.56245   2.46932   8.78356  L
H-HC-0.029500        0    -1.99239   1.6951    6.92527  L
H-HC-0.029500        0    -1.11547   0.18639   6.86144  L
H-HA-0.133000        0    -1.06545   3.78034   6.04038  L
H-HA-0.133000        0     1.00241   0.02486   5.65429  L
H-HA-0.143000        0     0.16017   4.66451   4.09996  L
H-HA-0.143000        0     2.32261   0.94216   3.75541  L
H-HA-0.129700        0     1.90461   3.2588    2.9675   L
N-N--0.415700        0    -1.36391  -0.17656   10.21887  L
C-CT--0.003100      -1    -2.22446  -1.02382   11.02576  L
C-C-0.597300         0    -3.45461  -0.31955   11.65194  L
O-O--0.567900        0    -4.59608  -0.69892   11.40579  L
C-CT--0.003600       0    -1.29133  -1.59895   12.113   L
C-CT--0.064500       0    -1.93528  -2.32477   13.30728  L
C-C-0.695100         0    -0.99121  -2.34264   14.50826  L
O-O--0.608600        0    -0.49609  -3.378     14.92548  L
N-N--0.940700        0    -0.7032   -1.21286   15.12369  L
H-H-0.271900         0    -0.36537  -0.27586   10.34607  L
H-H1-0.085000        0    -2.61157  -1.83626   10.42426  L
H-HC-0.017100        0    -0.70634  -0.76839   12.51119  L
H-HC-0.017100        0    -0.58781  -2.2819    11.63838  L
H-HC-0.035200        0    -2.18217  -3.34622   13.01691  L
H-HC-0.035200        0    -2.85112  -1.83333   13.62782  L
H-H-0.425100         0    -0.05725  -1.31045   15.87951  L
H-H-0.425100         0    -1.00807  -0.28626   14.81084  L
N-N--0.516300        0    -3.23261   0.63451   12.55242  L
C-CT-0.038100       -1    -4.24134   1.4592    13.25797  L
C-C-0.536600         0    -4.77715   2.58612   12.37129  L
O-O--0.581900        0    -5.92538   2.9993    12.52902  L
C-CT--0.030300       0    -3.60895   2.01297   14.5472  L
C-C-0.799400         0    -2.16145   2.43444   14.30117  L
O-O2--0.801400       0    -1.94979   3.51292   13.70764  L
O-O2--0.801400       0    -1.27337   1.5671    14.49487  L
H-H-0.293600         0    -2.25541   0.84425   12.72975  L
H-H1-0.088000        0    -5.09473   0.83858   13.53219  L
H-HC--0.012200       0    -3.62361   1.22861   15.30632  L
H-HC--0.012200       0    -4.19194   2.85653   14.92056  L
N-N--0.415700        0    -3.96896   3.0447    11.40953  L
C-CT-0.014300       -1    -4.34036   4.08487   10.45466  L
C-C-0.597300         0    -5.62794   3.7496    9.70365  L
O-O--0.567900        0    -6.46376   4.61788   9.45498  L
C-CT--0.204100       0    -3.20803   4.37432   9.43719  L
C-C-0.713000         0    -1.8263    4.79231   9.93336  L
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O-O--0.593100        0    -0.97788   5.17898   9.14383  L
N-N--0.919100        0    -1.4761    4.71244   11.19799  L
H-H-0.271900         0    -3.06515   2.60365   11.32525  L
H-H1-0.104800        0    -4.53745   5.00312   11.01065  L
H-HC-0.079700        0    -3.55455   5.18612   8.79532  L
H-HC-0.079700        0    -3.07566   3.52027   8.78111  L
H-H-0.419600         0    -0.55594   5.07443   11.35874  L
H-H-0.419600         0    -2.05157   4.39552   11.97911  L
N-N--0.347900        0    -5.78858   2.46447   9.37304  L
C-CT--0.263700       -1   -6.91507   1.93206   8.61244  L
C-C-0.734100         0    -8.32133   2.21427   9.16389  L
O-O--0.589400        0    -9.30752   1.96746   8.47093  L
C-CT--0.000700       0    -6.7012    0.43366   8.33132  L
C-CT-0.039000        0    -7.27876  -0.45921   9.43462  L
C-CT-0.048600        0    -6.85751  -1.91686   9.27364  L
N-N2--0.529500       0    -7.53667  -2.72219   10.29617  L
C-CA-0.807600        0    -7.03329  -3.09061   11.44919  L
N-N2--0.862700       0    -5.76271  -3.195     11.67729  L
N-N2--0.862700       0    -7.82231  -3.31062   12.45164  L
H-H-0.274700         0    -5.01146   1.85399   9.60272  L
H-H1-0.156000        0    -6.88872   2.43932   7.64499  L
H-HC-0.032700        0    -5.63366   0.23402   8.22027  L
H-HC-0.032700        0    -7.19582   0.1799    7.39221  L
H-HC-0.028500        0    -8.3684   -0.414     9.40556  L
H-HC-0.028500        0    -6.94199  -0.09739   10.40656  L
H-H1-0.068700        0    -5.77628  -1.97152   9.37716  L
H-H1-0.068700        0    -7.12934  -2.28008   8.28555  L
H-H-0.345600         0    -8.54529  -2.78177   10.23997  L
H-H-0.447800         0    -5.38905  -2.26307   11.81812  L
H-H-0.447800         0    -5.2816   -3.5265    10.83159  L
H-H-0.447800         0    -7.39687  -3.54198   13.32388  L
H-H-0.447800         0    -8.79646  -3.02787   12.34709  L
N-N--0.415700        0    -8.44324   2.6949    10.39807  L
C-CT--0.149000       -1   -9.72161   3.03847   10.98974  L
H-H-0.271900         0    -7.58531   2.89212   10.89916  L
H-H1-0.097600        0    -10.31074   3.6365    10.29348  L
H-H1-0.097600        0    -9.55926   3.60821   11.9054  L
H-H1-0.097600        0    -10.26712   2.12312   11.22812  L
C-CT--0.366200       -1   -9.9474    6.23994   8.78387  L
C-C-0.597200         0    -10.65993   5.48699   7.68561  L
O-O--0.567900        0    -11.84425   5.72345   7.48565  L
H-HC-0.112300        0    -9.13495   5.63619   9.18917  L
H-HC-0.112300        0    -10.65707   6.47882   9.57271  L
H-HC-0.112300        0    -9.53874   7.15876   8.36747  L
N-N--0.415700        0    -9.96453   4.57283   7.0053   L
C-CT--0.001400       -1   -10.48455   3.72456   5.91264  L
C-C-0.597300         0    -11.81442   3.01981   6.21843  L
O-O--0.567900        0    -12.69138   2.87669   5.36311  L
C-CT--0.015200       0    -9.34363   2.82906   5.37613  L
C-CA--0.001100       0    -9.72575   1.59028   4.58567  L
C-CA--0.190600       0    -10.34315   0.50691   5.23973  L
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C-CA--0.190600       0    -9.39625   1.48584   3.21942  L
C-CA--0.234100       0    -10.68303  -0.65047   4.51989  L
C-CA--0.234100       0    -9.69243   0.30871   2.5037   L
C-C-0.322600         0    -10.34698  -0.75525   3.15529  L
O-OH--0.557900       0    -10.67014  -1.88499   2.48199  L
H-H-0.271900         0    -8.99135   4.46301   7.25017  L
H-H1-0.087600        0    -10.7316   4.40032   5.09228  L
H-HC-0.029500        0    -8.7139    2.49806   6.19465  L
H-HC-0.029500        0    -8.70324   3.45534   4.75343  L
H-HA-0.169900        0    -10.56387   0.57295   6.29541  L
H-HA-0.169900        0    -8.89813   2.30621   2.72083  L
H-HA-0.165600        0    -11.18674  -1.46677   5.00825  L
H-HA-0.165600        0    -9.4359    0.21265   1.45721  L
H-HO-0.399200        0    -11.57742  -2.11886   2.74508  L
N-N--0.516300        0    -11.97967   2.60199   7.46609  L
C-CT-0.038100        -1   -13.20407   2.03136   8.00465  L
C-C-0.536600         0    -14.41316   2.98449   8.15696  L
O-O--0.581900        0    -15.54591   2.48417   8.20251  L
C-CT--0.030300       0    -12.87614   1.47726   9.41531  L
C-C-0.799400         0    -12.17166   0.11556   9.42541  L
O-O2--0.801400       0    -12.65813  -0.79799   8.72057  L
O-O2--0.801400       0    -11.20981  -0.09506   10.19156  L
H-H-0.293600         0    -11.14887   2.65519   8.04793  L
H-H1-0.088000        0    -13.5185   1.21013   7.36057  L
H-HC--0.012200       0    -13.80578   1.35259   9.9726   L
H-HC--0.012200       0    -12.28143   2.20977   9.96178  L
N-N--0.415700        0    -14.18144   4.29565   8.34126  L
C-CT--0.149000       -1   -15.13616   5.33453   8.75659  L
H-H-0.271900         0    -13.2284   4.60018   8.15756  L
H-H1-0.097600        0    -16.04035   5.26273   8.1501   L
H-H1-0.097600        0    -14.68599   6.3184    8.6132   L
H-H1-0.097600        0    -15.39436   5.2005    9.80735  L
C-CT--0.366200       -1   -19.75912  -1.28804  -1.32627  L
C-C-0.597200         0    -18.7713  -0.9217   -0.20702  L
O-O--0.567900        0    -18.40481   0.24324  -0.12176  L
H-HC-0.112300        0    -20.60422  -1.82808  -0.90673  L
H-HC-0.112300        0    -19.24279  -1.89954  -2.06489  L
H-HC-0.112300        0    -20.10529  -0.37174  -1.80271  L
N-N--0.415700        0    -18.32971  -1.86216   0.65776  L
C-CT--0.058100       -1   -17.20475  -1.63056   1.61391  L
C-C-0.597300         0    -16.35192  -2.85682   1.95303  L
O-O--0.567900        0    -16.77578  -3.6822    2.76705  L
C-CT--0.007400       0    -17.6463  -0.85475   2.86605  L
C-CC-0.186800        0    -16.46542  -0.1117    3.44728  L
N-NB--0.543200       0    -15.42018  -0.71264   4.14002  L
C-CW--0.220700       0    -16.1443   1.19758   3.22715  L
C-CR-0.163500        0    -14.46603   0.22498   4.28034  L
N-NA--0.279500       0    -14.89469   1.39615   3.78625  L
H-H-0.271900         0    -18.66896  -2.80388   0.54431  L
H-H1-0.136000        0    -16.55317  -0.92417   1.10473  L
H-HC-0.036700        0    -18.06352  -1.53479   3.60906  L
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H-HC-0.036700        0    -18.41054  -0.12474   2.59778  L
H-H4-0.186200        0    -16.72155   1.907     2.648    L
H-H-0.333900         0    -14.32877   2.24345   3.80479  L
H-H5-0.143500        0    -13.49479   0.07115   4.73714  L
N-N--0.254800        0    -15.14605  -2.97886   1.36745  L
C-CT--0.026600       -1   -14.1864   -3.9876    1.78263  L
C-C-0.589600         0    -13.5      -3.64866   3.09618  L
O-O--0.574800        0    -13.11556  -2.50355   3.33325  L
C-CT--0.007000       0    -13.13649  -4.02789   0.68069  L
C-CT-0.018900        0    -13.17175  -2.6381    0.04715  L
C-CT-0.019200        0    -14.61741  -2.19618   0.24898  L
H-H1-0.064100        0    -14.67074  -4.96162   1.86264  L
H-HC-0.025300        0    -13.45547  -4.77055  -0.03423  L
H-HC-0.025300        0    -12.14334  -4.27744   1.05756  L
H-HC-0.021300        0    -12.90124  -2.6618   -1.00887  L
H-HC-0.021300        0    -12.51032  -1.96315   0.58827  L
H-H1-0.039100        0    -14.62881  -1.12624   0.45878  L
H-H1-0.039100        0    -15.19411  -2.41257  -0.65177  L
N-N--0.347900        0    -13.224    -4.66274   3.91819  L
C-CT--0.263700       -1   -12.46105  -4.47393   5.15883  L
C-C-0.734100         0    -10.94923  -4.80833   4.9867   L
O-O--0.589400        0    -10.62009  -5.66584   4.17274  L
C-CT--0.000700       0    -13.17915  -5.12385   6.35409  L
C-CT-0.039000        0    -14.49936  -4.38101   6.6815   L
C-CT-0.048600        0    -14.28958  -2.99424   7.32908  L
N-N2--0.529500       0    -15.20717  -1.95606   6.80366  L
C-CA-0.807600        0    -15.62503  -0.85801   7.41842  L
N-N2--0.862700       0    -15.34178  -0.58467   8.65154  L
N-N2--0.862700       0    -16.30403   0.05501   6.79309  L
H-H-0.274700         0    -13.48215  -5.59284   3.61413  L
H-H1-0.156000        0    -12.44231  -3.40762   5.37492  L
H-HC-0.032700        0    -12.52959  -5.10206   7.23113  L
H-HC-0.032700        0    -13.39905  -6.16518   6.11527  L
H-HC-0.028500        0    -15.07977  -4.99215   7.37329  L
H-HC-0.028500        0    -15.0903   -4.27663   5.77032  L
H-H1-0.068700        0    -13.26919  -2.66066   7.14575  L
H-H1-0.068700        0    -14.40692  -3.09471   8.40958  L
H-H-0.345600         0    -15.39561  -1.96829   5.80626  L
H-H-0.447800         0    -15.57477   0.33884   8.97186  L
H-H-0.447800         0    -14.44657  -0.9929    8.92288  L
H-H-0.447800         0    -16.38314   0.97109   7.219    L
H-H-0.447800         0    -16.33847  -0.03546   5.78439  L
N-N--0.415700        0    -10.02773  -4.08722   5.65727  L
C-CT--0.003100       -1   -8.54092   -4.18439   5.54171  L
C-C-0.597300         0    -7.93855   -5.01406   6.68252  L
O-O--0.567900        0    -8.39664   -4.93756   7.82433  L
C-CT--0.003600       0    -7.91829   -2.78249   5.49828  L
C-CT--0.064500       0    -6.3851    -2.85268   5.39244  L
C-C-0.695100         0    -5.8052    -1.52604   4.95449  L
O-O--0.608600        0    -6.05748   -1.09814   3.84065  L
N-N--0.940700        0    -5.00447   -0.86833   5.75808  L
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H-H-0.271900          0    -10.37611  -3.39845   6.31424  L
H-H1-0.085000         0    -8.31261   -4.69409   4.61149  L
H-HC-0.017100         0    -8.19408   -2.22242   6.39023  L
H-HC-0.017100         0    -8.31791   -2.24787   4.63854  L
H-HC-0.035200         0    -6.09972   -3.59474   4.64768  L
H-HC-0.035200         0    -5.96361   -3.14365   6.35202  L
H-H-0.425100          0    -4.74603    0.08092   5.50744  L
H-H-0.425100          0    -4.67432   -1.32483   6.61804  L
N-N--0.415700         0    -6.87843   -5.76358   6.37438  L
C-CT--0.001400        -1   -6.12817   -6.57946   7.32432  L
C-C-0.597300          0    -4.62476   -6.5153    7.0335   L
O-O--0.567900         0    -4.18279   -6.69267   5.8923   L
C-CT--0.015200        0    -6.60349   -8.04446   7.26972  L
C-CA--0.001100        0    -8.09974   -8.24086   7.10628  L
C-CA--0.190600        0    -8.94409   -8.4089    8.22308  L
C-CA--0.190600        0    -8.64754   -8.20551   5.811    L
C-CA--0.234100        0    -10.33581  -8.55647   8.03937  L
C-CA--0.234100        0    -10.03255  -8.32736   5.63313  L
C-C-0.322600          0    -10.88056  -8.51936   6.73786  L
O-OH--0.557900        0    -12.21293  -8.67381   6.52616  L
H-H-0.271900          0    -6.59316   -5.80422   5.40045  L
H-H1-0.087600         0    -6.303     -6.19677   8.33107  L
H-HC-0.029500         0    -6.26949   -8.55304   8.17473  L
H-HC-0.029500         0    -6.11607   -8.53833   6.42735  L
H-HA-0.169900         0    -8.52584   -8.40836   9.21908  L
H-HA-0.169900         0    -8.00864   -8.03958   4.95302  L
H-HA-0.165600         0    -10.9991   -8.68513   8.87989  L
H-HA-0.165600         0    -10.455    -8.23886   4.65025  L
H-HO-0.399200         0    -12.35114  -8.7779    5.57239  L
N-N--0.516300         0    -3.82463   -6.27939   8.07081  L
C-CT-0.039700         -1   -2.37459   -6.19271   7.9428   L
C-C-0.536600          0    -1.67435   -7.56015   8.02443  L
O-O--0.581900         0    -1.88921   -8.3433    8.94976  L
C-CT-0.056000         0    -1.76363   -5.19792   8.93834  L
C-CT-0.013600         0    -2.03217   -3.74501   8.51669  L
C-C-0.805400          0    -3.51507   -3.34607   8.60338  L
O-O2--0.818800        0    -4.2092    -3.83118   9.53031  L
O-O2--0.818800        0    -3.96751   -2.55478   7.7472   L
H-H-0.293600          0    -4.23883   -5.96447   8.94051  L
H-H1-0.110500         0    -2.1698    -5.79694   6.95431  L
H-HC--0.017300        0    -0.68108   -5.33855   8.94486  L
H-HC--0.017300        0    -2.13276   -5.38734   9.9473   L
H-HC--0.042500        0    -1.67135   -3.60693   7.49534  L
H-HC--0.042500        0    -1.43418   -3.09522   9.15569  L
N-N--0.415700         0    -0.78528   -7.83817   7.06452  L
C-CT--0.002400        -1   -0.01933   -9.08757   6.96243  L
C-C-0.597300          0     1.4825    -8.84529   7.13656  L
O-O--0.567900         0     1.99473   -7.72172   7.16205  L
C-CT--0.034300        0    -0.36152   -9.77723   5.62229  L
C-CA-0.011800         0     0.18877   -9.08869   4.38069  L
C-CA--0.125600        0    -0.54883   -8.08334   3.73014  L
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C-CA--0.125600       0     1.46432  -9.42717   3.89367  L
C-CA--0.170400       0     0.0168   -7.37466   2.65331  L
C-CA--0.170400       0     2.03343  -8.71827   2.82016  L
C-CA--0.107200       0     1.30915  -7.68587   2.20237  L
H-H-0.271900         0    -0.65921  -7.13534   6.34069  L
H-H1-0.097800        0    -0.33747  -9.7532    7.76561  L
H-HC-0.029500        0    -1.44708  -9.85006   5.53308  L
H-HC-0.029500        0     0.01999  -10.79822   5.64845  L
H-HA-0.133000        0    -1.53258  -7.81344   4.09104  L
H-HA-0.133000        0     2.01283  -10.22672   4.36032  L
H-HA-0.143000        0    -0.52547  -6.55969   2.19478  L
H-HA-0.143000        0     3.02623  -8.95895   2.47343  L
H-HA-0.129700        0     1.74017  -7.11778   1.39107  L
N-N--0.415700        0     2.21956  -9.94433   7.27977  L
C-CT--0.024900       -1    3.66278  -9.89032   7.47252  L
C-C-0.597300         0     4.41603  -9.39541   6.22104  L
O-O--0.567900        0     4.2927   -9.95869   5.13562  L
C-CT-0.211700        0     4.21204  -11.26333   7.90004  L
O-OH--0.654600       0     3.97301  -12.29075   6.94399  L
H-H-0.271900         0     1.74066  -10.82698   7.21839  L
H-H1-0.084300        0     3.8647   -9.19149   8.28527  L
H-H1-0.035200        0     3.7579   -11.54792   8.85078  L
H-H1-0.035200        0     5.28849  -11.17358   8.05517  L
H-HO-0.427500        0     3.1928   -12.78249   7.23086  L
N-N--0.347900        0     5.27001  -8.37774   6.36613  L
C-CT--0.263700       -1    6.1515   -7.85356   5.29836  L
C-C-0.734100         0     7.25121  -8.83884   4.87169  L
O-O--0.589400        0     7.31826  -9.97444   5.34804  L
C-CT--0.000700       0     6.66441  -6.47404   5.77133  L
C-CT-0.039000        0     7.80762  -6.50606   6.7993   L
C-CT-0.048600        0     8.06467  -5.12994   7.43292  L
N-N2--0.529500       0     8.3497   -4.06816   6.44093  L
C-CA-0.807600        0     7.56513  -3.05511   6.10507  L
N-N2--0.862700       0     6.35322  -2.96269   6.55664  L
N-N2--0.862700       0     7.96444  -2.09429   5.32855  L
H-H-0.274700         0     5.26636  -7.92815   7.26831  L
H-H1-0.156000        0     5.52701  -7.68766   4.41746  L
H-HC-0.032700        0     5.8221   -5.9208    6.1917   L
H-HC-0.032700        0     7.0067   -5.90468   4.91737  L
H-HC-0.028500        0     8.72221  -6.84344   6.31384  L
H-HC-0.028500        0     7.56085  -7.20845   7.59602  L
H-H1-0.068700        0     8.92357  -5.22014   8.09954  L
H-H1-0.068700        0     7.20721  -4.86021   8.05094  L
H-H-0.345600         0     9.27754  -4.06975   6.02492  L
H-H-0.447800         0     5.7814   -2.14963   6.28987  L
H-H-0.447800         0     5.95898  -3.6302    7.17709  L
H-H-0.447800         0     7.26796  -1.36017   5.16439  L
H-H-0.447800         0     8.84756  -2.09301   4.84739  L
N-N--0.415700        0     8.12073  -8.39379   3.97419  L
C-CT--0.051800       -1    9.45132  -8.93489   3.70117  L
C-C-0.597300         0     10.38121  -7.73679   3.86474  L
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O-O--0.567900        0     10.44072  -6.85127   3.0167   L
C-CT--0.110200       0     9.45372   -9.56861   2.29376  L
C-CT-0.353100        0     10.7658   -10.24862   1.85006  L
C-CT--0.412100       0     10.45758  -11.27163   0.7538   L
C-CT--0.412100       0     11.79232  -9.2807    1.26366  L
H-H-0.271900         0     7.92974   -7.48297   3.56289  L
H-H1-0.092200        0     9.71367   -9.69898   4.43537  L
H-HC-0.045700        0     9.16046   -8.8275    1.54893  L
H-HC-0.045700        0     8.68362   -10.33323   2.30452  L
H-HC--0.036100       0     11.2054   -10.77294   2.69876  L
H-HC-0.100000        0     11.37733  -11.76809   0.44288  L
H-HC-0.100000        0     10.01786  -10.77021  -0.11079  L
H-HC-0.100000        0     9.76861   -12.02823   1.12593  L
H-HC-0.100000        0     12.66443  -9.8339    0.91651  L
H-HC-0.100000        0     12.11913  -8.56643   2.01086  L
H-HC-0.100000        0     11.35677  -8.73999   0.42443  L
N-N--0.415700        0     11.05689  -7.66761   5.00418  L
C-CT-0.014300        -1    12.32471  -6.96719   5.04355  L
C-C-0.597300         0     13.3883   -8.0144    4.62042  L
O-O--0.567900        0     13.42246  -9.07869   5.23805  L
C-CT--0.204100       0     12.63443  -6.44938   6.4586   L
C-C-0.713000         0     11.78212  -5.27942   6.9085   L
O-O--0.593100        0     11.09997  -4.60792   6.15053  L
N-N--0.919100        0     11.79632  -4.98582   8.18711  L
H-H-0.271900         0     10.97345  -8.44827   5.63749  L
H-H1-0.104800        0     12.34384  -6.13519   4.33775  L
H-HC-0.079700        0     13.67413  -6.11964   6.48003  L
H-HC-0.079700        0     12.52968  -7.26716   7.172    L
H-H-0.419600         0     11.27716  -4.17379   8.46198  L
H-H-0.419600         0     12.39098  -5.50096   8.81521  L
N-N--0.415700        0     14.19292  -7.78484   3.5715   L
C-CT--0.051800       -1    15.30392  -8.68675   3.20958  L
C-C-0.597300         0     16.51677  -8.4521    4.14908  L
O-O--0.567900        0     16.78117  -7.31061   4.52297  L
C-CT--0.110200       0     15.66954  -8.54702   1.69771  L
C-CT-0.353100        0     16.69706  -9.57084   1.12933  L
C-CT--0.412100       0     16.21582  -11.0135   1.32376  L
C-CT--0.412100       -1    16.97926  -9.41637  -0.38542  L
H-H-0.271900         0     14.1267   -6.90886   3.07416  L
H-H1-0.092200        0     14.95993  -9.70667   3.37742  L
H-HC-0.045700        0     16.06371  -7.54565   1.52871  L
H-HC-0.045700        0     14.75395  -8.63481   1.11408  L
H-HC--0.036100       0     17.6395   -9.44935   1.65859  L
H-HC-0.100000        0     15.24041  -11.14942   0.85712  L
H-HC-0.100000        0     16.15279  -11.25534   2.38214  L
H-HC-0.100000        0     16.93011  -11.70076   0.86948  L
H-HC-0.100000        0     16.08439  -9.64533  -0.96023  L
H-HC-0.100000        0     17.78437  -10.0897  -0.67959  L
H-HC-0.100000        0     17.29622  -8.39204  -0.58528  L
N-N--0.516300        0     17.24888  -9.50505   4.54558  L
C-CT-0.039700        -1    18.50164  -9.36788   5.32725  L
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C-C-0.536600          0     19.58059  -8.55909   4.54937  L
O-O--0.581900         0     19.5126  -8.43656   3.3232   L
C-CT-0.056000         0     19.04129  -10.73326   5.7949   L
C-CT-0.013600         0     18.74163  -10.98761   7.28258  L
C-C-0.805400          0     19.28411  -9.88712   8.21699  L
O-O2--0.818800        0     18.73968  -9.76696   9.33437  L
O-O2--0.818800        0     20.18532  -9.12923   7.78139  L
H-H-0.293600          0     16.99859  -10.42168   4.21956  L
H-H1-0.110500         0     18.26291  -8.76006   6.20078  L
H-HC--0.017300        0     20.12182  -10.77345   5.64919  L
H-HC--0.017300        0     18.60195  -11.53296   5.19579  L
H-HC--0.042500        0     19.17924  -11.94804   7.56388  L
H-HC--0.042500        0     17.65817  -11.06632   7.40251  L
N-N--0.415700         0     20.54257  -7.93261   5.24535  L
C-CT--0.025200        -1    21.54357  -6.99299   4.67807  L
C-C-0.597300          0     20.92034  -5.72786   4.02215  L
O-O--0.567900         0     21.6639  -4.95091   3.42712  L
H-H-0.271900          0     20.56432  -8.14738   6.24674  L
H-H1-0.069800         0     22.1281  -7.51211   3.91867  L
H-H1-0.069800         0     22.21824  -6.66945   5.46978  L
N-N--0.415700         0     19.59275  -5.48762   4.09889  L
C-CT--0.038900        0     18.85467  -4.58835   3.17122  L
C-C-0.597300          0     17.88785  -3.58806   3.8481   L
O-O--0.567900         0     17.07538  -3.93354   4.70356  L
C-CT-0.365400         0     18.06098  -5.41557   2.13722  L
O-OH--0.676100        0     18.83867  -6.4368    1.55359  L
C-CT--0.243800        0     17.58545  -4.57421   0.9511   L
H-H-0.271900          0     19.03883  -6.15324   4.62278  L
H-H1-0.100700         0     19.58828  -4.01      2.611    L
H-H1-0.004300         0     17.19142  -5.85822   2.6162   L
H-HC-0.064200         0     16.9185  -3.78225   1.28209  L
H-HC-0.064200         0     17.04417  -5.21381   0.25369  L
H-HC-0.064200         0     18.44363  -4.13947   0.43804  L
H-HO-0.410200         0     19.07294  -7.09185   2.23824  L
N-N--0.415700         0     17.91822  -2.31902   3.4152   L
C-CT--0.087500        -1    17.00344  -1.21864   3.81685  L
C-C-0.597300          0     15.64132  -1.36697   3.10178  L
O-O--0.567900         0     15.59802  -1.39719   1.87549  L
C-CT-0.298500         0     17.59092   0.15445   3.4068   L
C-CT--0.319200        -1    16.71532   1.35326   3.87142  L
C-CT--0.319200        -1    19.03599   0.26247   3.92698  L
H-H-0.271900          0     18.59039  -2.11701   2.69025  L
H-H1-0.096900         0     16.85959  -1.24397   4.89627  L
H-HC--0.029700        0     17.64987   0.20078   2.31903  L
H-HC-0.079100         0     16.59187   1.33193   4.9532   L
H-HC-0.079100         0     15.74271   1.33123   3.38025  L
H-HC-0.079100         0     17.21699   2.27907   3.59085  L
H-HC-0.079100         0     19.0623   0.0929    5.00351  L
H-HC-0.079100         0     19.42032   1.26136   3.718    L
H-HC-0.079100         0     19.69008  -0.45201   3.4278   L
N-N--0.415700         0     14.51832  -1.47039   3.83211  L
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 C-CT--0.023700       -1    13.21921  -1.91854   3.26324  L
 C-C-0.597300         0     11.94128  -1.27288   3.88461  L
 O-O--0.567900        0     10.82855  -1.79985   3.76514  L
 C-CT-0.034200        0     13.11432  -3.44694   3.51157  L
 C-CT-0.001800        0     14.2035  -4.35977   2.92424  L
 S-S--0.273700        0     13.73507  -5.25909   1.42153  L
 C-CT--0.053600       0     13.82134  -3.9128    0.21642  L
 H-H-0.271900         0     14.65565  -1.53185   4.82814  L
 H-H1-0.088000        0     13.18931  -1.73083   2.18928  L
 H-HC-0.024100        0     12.15554  -3.81384   3.14258  L
 H-HC-0.024100        0     13.11798  -3.59983   4.59147  L
 H-H1-0.044000        0     14.45248  -5.09983   3.684    L
 H-H1-0.044000        0     15.11687  -3.80763   2.73066  L
 H-H1-0.068400        0     14.81392  -3.46245   0.23059  L
 H-H1-0.068400        0     13.07847  -3.15312   0.45453  L
 H-H1-0.068400        0     13.62218  -4.31345  -0.77489  L
 N-N--0.415700        0     12.06778  -0.12508   4.5571   L
 C-CT--0.024900       -1    10.95254   0.80589   4.83982  L
 C-C-0.597300         0     11.04283   1.88598   3.76643  L
 O-O--0.567900        0     12.14113   2.39466   3.53466  L
 C-CT-0.211700        0     11.08503   1.36586   6.25453  L
 O-OH--0.654600       0     10.15066   2.38924   6.52506  L
 H-H-0.271900         0     12.98887   0.28693   4.51528  L
 H-H1-0.084300        0     9.99041   0.29964   4.75061  L
 H-H1-0.035200        0     12.08803   1.76831   6.37961  L
 H-H1-0.035200        0     10.94519   0.55501   6.97062  L
 H-HO-0.427500        0     9.24717   2.07602   6.38109  L
 N-N--0.347900        0     9.9497    2.18062   3.04956  L
 C-CT--0.240000       -1    9.99178   3.10524   1.90447  L
 C-C-0.734100         0     10.5399   4.4809    2.34381  L
 O-O--0.589400        0     11.55862   4.88053   1.78465  L
 C-CT--0.009400       0     8.60921   3.16231   1.23123  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.56994   3.9685   -0.08224  H
 C-CT--0.047900       0     7.27824   3.59917  -0.81602  H
 C-CT--0.014300       0     7.01161   4.38828  -2.08796  H
 N-N3--0.385400       0     5.6691    3.97273  -2.66815  H
 H-H-0.274700         0     9.05941   1.7456    3.28334  L
 H-H1-0.142600        0     10.70128   2.71517   1.17316  L
 H-HC-0.036200        0     7.87798   3.57838   1.92356  L
 H-HC-0.036200        0     8.30886   2.13496   1.01477  L
 H-HC-0.010300        0     9.45154   3.72507  -0.68284  H
 H-HC-0.010300        0     8.58799   5.03132   0.17356  H
 H-HC-0.062100        0     6.41995   3.75851  -0.16027  H
 H-HC-0.062100        0     7.27647   2.53668  -1.07907  H
 H-HP-0.113500        0     7.73802   4.21676  -2.88759  H
 H-HP-0.113500        0     6.9405    5.46064  -1.91125  H
 H-H-0.340000         0     5.78784   3.24159  -3.38354  H
 H-H-0.340000         0     5.22844   4.73258  -3.2241   H
 H-H-0.340000         0     5.00817   3.61519  -1.95074  H
 N-N--0.347900        0     10.02914   5.11214   3.42821  L
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C-CT--0.263700       -1    10.62509   6.30809   4.12128  L
C-C-0.734100         0     11.86409   6.01142   4.9576   L
O-O--0.589400        0     12.06233   6.56374   6.03649  L
C-CT--0.000700       0     9.51953   7.17372   4.7711   L
C-CT-0.039000        0     8.64589   7.7786    3.64758  L
C-CT-0.048600        0     7.59747   8.82275   4.05628  L
N-N2--0.529500       0     6.51712   8.27625   4.8953   L
C-CA-0.807600        0     5.28138   8.73245   5.01144  L
N-N2--0.862700       0     4.76615   9.61551   4.20372  L
N-N2--0.862700       0     4.56035   8.29356   5.99475  L
H-H-0.274700         0     9.16934   4.72064   3.79961  L
H-H1-0.156000        0     11.04929   6.93614   3.33268  L
H-HC-0.032700        0     9.97601   7.99085   5.33175  L
H-HC-0.032700        0     8.91332   6.56994   5.4473   L
H-HC-0.028500        0     8.14147   6.97414   3.12387  L
H-HC-0.028500        0     9.30534   8.26763   2.92938  L
H-H1-0.068700        0     7.16951   9.23349   3.13959  L
H-H1-0.068700        0     8.09236   9.63438   4.59196  L
H-H-0.345600         0     6.73058   7.52415   5.53946  L
H-H-0.447800         0     3.79902   9.9225    4.29603  L
H-H-0.447800         0     5.26618   9.87875   3.37182  L
H-H-0.447800         0     3.65204   8.70781   6.20596  L
H-H-0.447800         0     4.93371   7.57518   6.59083  L
N-N--0.347900        0     12.71834   5.1635    4.37401  L
C-CT--0.240000       -1    14.12307   4.87015   4.68296  L
C-C-0.734100         0     14.98179   4.5437    3.43127  L
O-O--0.589400        0     16.20029   4.61223   3.53358  L
C-CT--0.009400       0     14.27097   3.78151   5.77255  L
C-CT-0.018700        0     13.52408   4.18381   7.05443  L
C-CT--0.047900       0     13.7727   3.33879   8.30363  L
C-CT--0.014300       0     12.81518   3.90594   9.36447  L
N-N3--0.385400       0     12.97504   3.26415   10.69114  L
H-H-0.274700         0     12.36337   4.83984   3.48592  L
H-H1-0.142600        0     14.56361   5.78677   5.08049  L
H-HC-0.036200        0     15.33081   3.66642   6.00571  L
H-HC-0.036200        0     13.89494   2.82802   5.40466  L
H-HC-0.010300        0     12.45436   4.14648   6.8484   L
H-HC-0.010300        0     13.80457   5.20905   7.30091  L
H-HC-0.062100        0     14.81259   3.44842   8.61697  L
H-HC-0.062100        0     13.54741   2.29129   8.10128  L
H-HP-0.113500        0     11.78802   3.77971   9.00285  L
H-HP-0.113500        0     12.99487   4.98361   9.44661  L
H-H-0.340000         0     12.78463   2.27329   10.6306  L
H-H-0.340000         0     12.32521   3.67565   11.35084  L
H-H-0.340000         0     13.91502   3.40367   11.03836  L
N-N--0.415700        0     14.38969   4.18765   2.27882  L
C-CT--0.051800       -1    15.05281   3.74837   1.02261  L
C-C-0.597300         0     15.26463   4.84225   0.01026  L
O-O--0.567900        0     16.23803   4.81834  -0.74073  L
C-CT--0.110200       0     14.21125   2.58135   0.46262  L
C-CT-0.353100        0     14.7567   1.90193  -0.80877  L
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C-CT--0.412100       0     16.14889   1.30252  -0.60486  L
C-CT--0.412100       0     13.81117   0.769    -1.21685  L
H-H-0.271900         0     13.37949   4.15735   2.28336  L
H-H1-0.092200        0     16.04183   3.36569   1.27908  L
H-HC-0.045700        0     13.20974   2.95588   0.24418  L
H-HC-0.045700        0     14.11791   1.82221   1.24125  L
H-HC--0.036100       0     14.79358   2.62493  -1.62295  L
H-HC-0.100000        0     16.1406   0.60556   0.23212  L
H-HC-0.100000        0     16.87182   2.09502  -0.41402  L
H-HC-0.100000        0     16.45755   0.77543  -1.50723  L
H-HC-0.100000        0     14.16377   0.31703  -2.1437   L
H-HC-0.100000        0     12.80942   1.16528  -1.38033  L
H-HC-0.100000        0     13.77851   0.00743  -0.43658  L
N-N--0.415700        0     14.35832   5.80488   0.00164  L
C-CT-0.014300       -1     14.55521   7.01785  -0.74573  L
C-C-0.597300         0     15.62945   7.95202  -0.11429  L
O-O--0.567900        0     15.33092   9.04885   0.35098  L
C-CT--0.204100       0     13.18568   7.69039  -1.02245  L
C-C-0.713000         0     12.2119   7.79451   0.1483   L
O-O--0.593100        0     12.54072   7.65966   1.3177   L
N-N--0.919100        0     10.94426   7.98914  -0.13979  L
H-H-0.271900         0     13.60541   5.7849    0.67942  L
H-H1-0.104800        0     14.95659   6.75065  -1.72496  L
H-HC-0.079700        0     12.68694   7.11719  -1.80336  L
H-HC-0.079700        0     13.35352   8.69486  -1.4095   L
H-H-0.419600         0     10.32572   8.02397   0.64454  L
H-H-0.419600         0     10.59496   8.07868  -1.09242  L
N-N--0.415700        0     16.90303   7.52198  -0.15335  L
C-CT--0.149000      -1     18.09308   8.22879   0.33862  L
H-H-0.271900         0     17.02066   6.58725  -0.53097  L
H-H1-0.097600        0     18.03047   8.336     1.42295  L
H-H1-0.097600        0     18.1402   9.22304  -0.10952  L
H-H1-0.097600        0     18.99398   7.67076   0.08085  L
C-CT--0.055800       0     0.69445   15.28133   4.41955  L
C-CT-0.000000        0     1.05149   14.35394   3.2598   L
O-OS--0.354800       0     2.44727   14.41824   2.9992   L
C-CT--0.202200       0     0.74381   12.89343   3.59904  L
O-OS--0.524600       0     0.19478   12.31615   2.41283  L
C-CT--0.067000       0     2.12708   12.35781   3.95636  L
O-OH--0.613900       0     2.20713   10.95381   3.86406  L
C-CT--0.006600       0     2.90185   13.08294   2.87303  L
N-N*--0.048400       0     4.37037   12.94582   3.0323   L
C-C-0.753800         0     5.05091   12.06693   2.18464  L
O-O--0.625200        0     4.47692   11.47907   1.27191  L
N-NC--0.758400       0     6.37315   11.81933   2.37238  L
C-CA-0.818500        0     6.99791   12.46643   3.32818  L
N-N2--0.953000       0     8.27531   12.22607   3.4027   L
C-CM--0.521500       0     6.36885   13.369    4.22445  L
C-CM--0.005300       0     5.03967   13.58155   4.04841  L
H-H1-0.067900        0    -0.38415   15.25662   4.57712  L
H-H1-0.067900        0     1.19892   14.944    5.32468  L
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 H-H1-0.117400        0     0.47276   14.64603   2.37878  L
 H-H1-0.061500        0     0.03668   12.83448   4.42664  L
 H-H1-0.097200        0     2.42982   12.71233   4.94449  L
 H-HO-0.418600        0     1.56582   10.693    3.17125  L
 H-H2-0.202900        0     2.57537   12.67398   1.91176  L
 H-H-0.423400         0     8.62063   11.67815   2.63739  L
 H-H-0.423400         0     8.84541   12.75228   4.03372  L
 H-HA-0.192800        0     6.89501   13.87959   5.0131   L
 H-H4-0.195800        0     4.48827   14.25367   4.69646  L
 P-P-1.166200         0    -0.77448   11.02438   2.39224  L
 O-O2--0.776000       0    -1.67983   11.06587   1.22894  L
 O-O2--0.776000       0    -1.31649   10.77114   3.74582  L
 O-OS--0.498900       0     0.3102    9.88343   2.11919  L
 C-CT-0.055800        0     1.03165   9.82433   0.89761  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     1.72488   8.45886   0.77742  H
 O-OS--0.354800       0     2.57033   8.30017   1.90504  H
 C-CT-0.202200        0     0.77054   7.26202   0.79444  H
 O-OH--0.654100       0     0.23788   6.90378  -0.45781  H
 C-CT-0.067000        0     1.67405   6.14996   1.35771  H
 O-OH--0.613900       0     2.40037   5.55804   0.32388  H
 C-CT-0.039400        0     2.61016   6.94449   2.30035  H
 N-N*--0.025100       0     2.22228   6.83906   3.69425  H
 C-CK-0.200600        0     1.16754   7.43605   4.36125  H
 N-NB--0.607300       0     1.03676   7.02693   5.5969   H
 C-CB-0.051500        0     2.03366   6.08726   5.75676  H
 C-CA-0.700900        0     2.41931   5.24939   6.82638  H
 N-N2--0.901900       0     1.80981   5.26481   8.0422   H
 N-NC--0.761500       0     3.51551   4.48324   6.67453  H
 C-CQ-0.587500        0     4.08309   4.40934   5.47182  H
 N-NC--0.699700       0     3.81387   5.13213   4.38925  H
 C-CB-0.305300        0     2.77752   5.95647   4.58561  H
 H-H1-0.067900        0     1.77381   10.62262   0.87263  L
 H-H1-0.067900        0     0.35015   9.95066   0.05465  L
 H-H1-0.117400        0     2.30138   8.41712  -0.16327  H
 H-H1-0.061500        0    -0.03837   7.44226   1.51693  H
 H-HO-0.437600        0     0.00461   7.69782  -0.96684  H
 H-H1-0.097200        0     1.08779   5.4156    1.92675  H
 H-HO-0.418600        0     3.11511   5.00271   0.7028   H
 H-H2-0.200700        0     3.63466   6.57153   2.21144  H
 H-H5-0.155300        0     0.55473   8.18914   3.87777  H
 H-H-0.411500         0     1.9146    4.39057   8.56624  H
 H-H-0.411500         0     0.83022   5.55504   8.06467  H
 H-H5-0.047300        0     4.94009   3.75085   5.3764   H
 N-N3-0.149300        0     0.01421   4.13132  -0.72674  H
 C-CT-0.053600        0     0.52034   3.04672   0.12603  H
 C-CT-0.065100        0    -0.4813    1.86457   0.11033  H
 C-CT--0.090300       0    -0.45835   0.96613   1.35337  H
 C-C-0.735400         0    -1.50152  -0.14398   1.23568  H
 O-O--0.613300        0    -1.21659  -1.31537   1.06579  H
 N-N--1.003100        0    -2.80309   0.30263   1.20848  H
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 C-C-0.612300          0     1.86842   2.59708  -0.41647  H
 O-O--0.571300         0     2.25783   2.84856  -1.52881  H
 O-OS--0.421200        0     2.5487    1.82993   0.4529   H
 P-P-1.166200          0     4.15515   1.33036   0.26056  H
 O-O2--0.776000        0     4.74264   1.3898    1.63618  H
 O-O2--0.776000        0     4.82642   2.03466  -0.88118  H
 O-OS--0.498900        0     3.95396  -0.21024  -0.11847  H
 C-CT-0.055800         0     3.22674  -0.58827  -1.2922   H
 C-CT-0.106500         0     2.61042  -1.9814   -1.05755  L    H-H1
1624  0.        0.
 O-OS--0.354800        0     3.56543  -2.94505  -0.60287  L
 C-CT-0.039400         0     3.39123  -3.14226   0.80487  L
 N-N*--0.025100        0     4.70631  -3.07117   1.49242  L
 C-CB-0.305300         0     5.49424  -4.16046   1.76791  L
 N-NC--0.699700        0     5.17413  -5.46995   1.56974  L
 C-CQ-0.587500         0     6.15008  -6.27927   1.94304  L
 N-NC--0.761500        0     7.33836  -5.96467   2.44202  L
 C-CA-0.700900         0     7.62583  -4.66989   2.57636  L
 N-N2--0.901900        0     8.8546   -4.45196   3.00962  L
 C-CB-0.051500         0     6.67346  -3.67215   2.26491  L
 N-NB--0.607300        0     6.64287  -2.27714   2.35498  L
 C-CK-0.200600         0     5.43545  -1.9864    1.93053  L
 C-CT-0.067000         0     2.31537  -2.17133   1.30152  L
 O-OH--0.613900        0     1.53397  -2.71524   2.35007  L
 C-CT-0.202200         0     1.52237  -1.96038   0.0071   L
 O-OH--0.654100        0     0.60266  -3.02332  -0.21831  L
 H-H-0.199600          0    -1.24127   3.57419  -1.83773  H
 H-H-0.199600          0     0.79163   4.7014   -1.0615   H
 H-H-0.199600          0    -0.53548   4.77968  -0.16569  H
 H-HP-0.101500         0     0.6886    3.37691   1.16154  H
 H-HC-0.005000         0    -0.30927   1.27427  -0.79624  H
 H-HC-0.005000         0    -1.4798    2.29448  -0.00599  H
 H-HC-0.033100         0    -0.67634   1.57025   2.24444  H
 H-HC-0.033100         0     0.5154    0.50057   1.50271  H
 H-H-0.442900          0    -3.51369  -0.38716   1.40173  H
 H-H-0.442900          0    -2.97962   1.18525   1.69864  H
 H-H1-0.067900         0     3.90482  -0.63252  -2.14955  H
 H-H1-0.067900         0     2.42439   0.12144  -1.51704  H
 H-H1-0.117400         0     2.15892  -2.30039  -1.99623  L
 H-H2-0.200700         0     2.98169  -4.141     0.96263  L
 H-H5-0.047300         0     5.94891  -7.33372   1.82797  L
 H-H-0.411500          0     9.20865  -3.50983   3.05555  L
 H-H-0.411500          0     9.46125  -5.26553   3.05019  L
 H-H5-0.155300         0     5.06068  -0.97472   1.88921  L
 H-H1-0.097200         0     2.74991  -1.22512   1.62145  L
 H-HO-0.418600         0     2.0686   -2.72065   3.169    L
 H-H1-0.061500         0     1.0081   -1.00226  -0.00136  L
 H-HO-0.437600         0    -0.15421  -2.78546   0.35604  L
 O-OW--0.834000        0    -10.27811  -2.15361   11.56203  L
 H-HW-0.417000         0    -10.60694  -1.30908   11.16911  L
 H-HW-0.417000         0    -10.54172  -2.80389   10.88658  L
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O-OW--0.834000       0    -10.22197  -3.88928   9.47017  L
H-HW-0.417000        0    -10.47792  -3.2442    8.78288  L
H-HW-0.417000        0    -9.58897  -4.4566    8.98892  L
O-OW--0.834000       0    -10.68561  -2.00248   7.61024  L
H-HW-0.417000        0    -11.47803  -1.59354   8.04356  L
H-HW-0.417000        0    -10.05922  -1.27059   7.62937  L
O-OW--0.834000       0     4.17082   4.08422   1.87112  H
H-HW-0.417000        0     4.01237   4.41932   2.7826   H
H-HW-0.417000        0     4.30731   3.11842   1.91303  H
O-OW--0.834000       0     7.03761   4.3371    4.40603  H
H-HW-0.417000        0     6.84959   3.42839   4.10795  H
H-HW-0.417000        0     6.61631   4.89313   3.71929  H
O-OW--0.834000       0     6.61029   2.7179   -5.04147  L
H-HW-0.417000        0     7.35903   2.3824   -5.56802  L
H-HW-0.417000        0     6.41499   3.57268  -5.45211  L
O-OW--0.834000       0     6.38904   5.94058   6.63541  L
H-HW-0.417000        0     5.71841   5.42782   7.10821  L
H-HW-0.417000        0     6.67409   5.33003   5.93011  L
O-OW--0.834000       0     6.91183   1.41661   3.79021  H
H-HW-0.417000        0     6.2357    1.34773   3.08694  H
H-HW-0.417000        0     6.48001   0.90377   4.51408  H
O-OW--0.834000       0     6.27287   5.79677   2.01708  H
H-HW-0.417000        0     6.11279   6.5847    1.47086  H
H-HW-0.417000        0     5.60601   5.19108   1.63661  H
O-OW--0.834000       0     3.64137   16.66617   4.03811  L
H-HW-0.417000        0     3.22447   15.87689   3.65781  L
H-HW-0.417000        0     2.9245    17.29992   4.07088  L
O-OW--0.834000       0    -4.35212   2.0194    5.42726  L
H-HW-0.417000        0    -4.07967   2.19524   6.33255  L
H-HW-0.417000        0    -5.03121   2.73385   5.29124  L
O-OW--0.834000       0    -0.09324   1.90054   12.1231  L
H-HW-0.417000        0    -0.34686   1.78812   13.06184  L
H-HW-0.417000        0    -0.31975   2.82119   11.9651  L
O-OW--0.834000       0    -2.41984   9.49892   5.74442  L
H-HW-0.417000        0    -1.64806   9.62132   6.3079   L
H-HW-0.417000        0    -2.12725   9.92232   4.90459  L
O-OW--0.834000       0     2.08928   9.19555   6.99673  L
H-HW-0.417000        0     1.59456   8.38463   6.7812   L
H-HW-0.417000        0     1.42239   9.88266   6.80084  L
O-OW--0.834000       0    -5.12489   9.48966   5.30303  L
H-HW-0.417000        0    -5.2721    8.9957    6.12579  L
H-HW-0.417000        0    -4.16397   9.63856   5.33962  L
O-OW--0.834000       0    -4.408     7.89712   7.44823  L
H-HW-0.417000        0    -4.61064   6.98744   7.12018  L
H-HW-0.417000        0    -3.55532   8.08435   7.04255  L
O-OW--0.834000       0     0.24122   10.7874   5.8555   L
H-HW-0.417000        0     1.00085   11.08795   5.32934  L
H-HW-0.417000        0    -0.46635   10.84307   5.17573  L
O-O2--0.818800       0     5.04559   7.82686  -0.11049  H
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**TS1**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.54311 | -11.69969 | -5.50411 | L |
| C-C-0.597200 | 0 | -11.86545 | -10.68436 | -6.39516 | L |
| O-O--0.567900 | 0 | -11.48139 | -11.03536 | -7.50193 | L |
| H-HC-0.112300 | 0 | -11.93522 | -11.85282 | -4.61529 | L |
| H-HC-0.112300 | 0 | -12.6309 | -12.6373 | -6.05081 | L |
| H-HC-0.112300 | 0 | -13.53335 | -11.3362 | -5.23859 | L |
| N-N--0.415700 | 0 | -11.68885 | -9.46038 | -5.88848 | L |
| C-CT--0.058100 | -1 | -10.83023 | -8.43031 | -6.49263 | L |
| C-C-0.597300 | 0 | -9.80591 | -7.90889 | -5.4791 | L |
| O-O--0.567900 | 0 | -10.08013 | -7.83954 | -4.27463 | L |
| C-CT--0.007400 | 0 | -11.64222 | -7.33252 | -7.17473 | L |
| C-CC-0.186800 | 0 | -11.04546 | -6.85117 | -8.47103 | L |
| N-NB--0.543200 | 0 | -11.44471 | -7.25895 | -9.74347 | L |
| C-CW--0.220700 | 0 | -10.17261 | -5.81272 | -8.58801 | L |
| C-CR-0.163500 | 0 | -10.85681 | -6.40669 | -10.59592 | L |
| N-NA--0.279500 | 0 | -10.09031 | -5.52723 | -9.93207 | L |
| H-H-0.271900 | 0 | -12.05721 | -9.25904 | -4.9748 | L |
| H-H1-0.136000 | 0 | -10.26063 | -8.91959 | -7.28492 | L |
| H-HC-0.036700 | 0 | -11.70496 | -6.48336 | -6.50391 | L |
| H-HC-0.036700 | 0 | -12.6517 | -7.68939 | -7.38368 | L |
| H-H4-0.186200 | 0 | -9.74397 | -5.23853 | -7.78177 | L |
| H-H-0.333900 | 0 | -9.73893 | -4.65016 | -10.33588 | L |
| H-H5-0.143500 | 0 | -11.03797 | -6.3784 | -11.66094 | L |
| N-N--0.415700 | 0 | -8.61551 | -7.56965 | -5.9678 | L |
| C-CT--0.038900 | -1 | -7.4565 | -7.06384 | -5.21091 | L |
| C-C-0.597300 | 0 | -6.68853 | -5.98201 | -6.00694 | L |
| O-O--0.567900 | 0 | -7.03506 | -5.67782 | -7.14791 | L |
| C-CT-0.365400 | 0 | -6.46531 | -8.19287 | -4.85775 | L |
| O-OH--0.676100 | 0 | -6.18565 | -8.97778 | -5.97803 | L |
| C-CT--0.243800 | -1 | -6.97292 | -9.13425 | -3.78249 | L |
| H-H-0.271900 | 0 | -8.46329 | -7.76296 | -6.95166 | L |
| H-H1-0.100700 | 0 | -7.78174 | -6.63278 | -4.27178 | L |
| H-H1-0.004300 | 0 | -5.5338 | -7.76036 | -4.49251 | L |
| H-HC-0.064200 | 0 | -7.24411 | -8.56618 | -2.89253 | L |
| H-HC-0.064200 | 0 | -6.19282 | -9.84842 | -3.52355 | L |
| H-HC-0.064200 | 0 | -7.84974 | -9.6717 | -4.14459 | L |
| H-HO-0.410200 | 0 | -5.46688 | -9.59656 | -5.77038 | L |
| N-N--0.347900 | 0 | -5.61584 | -5.39644 | -5.43909 | L |
| C-CT--0.263700 | -1 | -4.63026 | -4.54985 | -6.16057 | L |
| C-C-0.734100 | 0 | -3.22608 | -4.62246 | -5.57539 | L |
| O-O--0.589400 | 0 | -3.10229 | -4.87274 | -4.3825 | L |
| C-CT--0.000700 | 0 | -5.12384 | -3.09512 | -6.27596 | L |
| C-CT-0.039000 | 0 | -4.89482 | -2.18811 | -5.05452 | L |
| C-CT-0.048600 | 0 | -5.70237 | -2.51216 | -3.79738 | L |
| N-N2--0.529500 | 0 | -5.09486 | -3.56105 | -2.97223 | L |
| C-CA-0.807600 | 0 | -5.08458 | -3.62908 | -1.66055 | L |
| N-N2--0.862700 | 0 | -5.78394 | -2.85655 | -0.8838 | L |
| N-N2--0.862700 | 0 | -4.31876 | -4.51558 | -1.10808 | L |
| H-H-0.274700 | 0 | -5.38546 | -5.69303 | -4.50281 | L |
| H-H1-0.156000 | 0 | -4.57431 | -4.95675 | -7.16665 | L |

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 H-HC-0.032700        0    -6.18347  -3.08549  -6.53615  L
 H-HC-0.032700        0    -4.59413  -2.63851  -7.11342  L
 H-HC-0.028500        0    -5.19013  -1.191    -5.35271  L
 H-HC-0.028500        0    -3.83661  -2.13886  -4.81033  L
 H-H1-0.068700        0    -6.71217  -2.79647  -4.08844  L
 H-H1-0.068700        0    -5.74499  -1.59614  -3.20648  L
 H-H-0.345600         0    -4.44126  -4.1789   -3.42978  L
 H-H-0.447800         0    -5.81759  -2.96846   0.11842  L
 H-H-0.447800         0    -6.52751  -2.26927  -1.28621  L
 H-H-0.447800         0    -4.02538  -4.35998  -0.14996  L
 H-H-0.447800         0    -3.86985  -5.22108  -1.68363  L
 N-N--0.415700        0    -2.18121  -4.29526  -6.33046  L
 C-CT--0.002400      -1    -0.93807  -3.77586  -5.73576  L
 C-C-0.597300         0    -1.01214  -2.23808  -5.67962  L
 O-O--0.567900        0    -1.093    -1.63176  -6.75123  L
 C-CT--0.034300       0     0.28424  -4.25552  -6.52634  L
 C-CA-0.011800        0     1.59319  -3.6746   -6.01636  L
 C-CA--0.125600       0     2.01898  -3.91274  -4.69308  L
 C-CA--0.125600       0     2.38251  -2.87479  -6.86352  L
 C-CA--0.170400       0     3.20808  -3.32697  -4.21954  L
 C-CA--0.170400       0     3.57265  -2.29754  -6.3922   L
 C-CA--0.107200       0     3.97189  -2.50212  -5.06354  L
 H-H-0.271900         0    -2.37943  -4.12974  -7.31304  L
 H-H1-0.097800        0    -0.82237  -4.17015  -4.72829  L
 H-HC-0.029500        0     0.15349  -3.98735  -7.57617  L
 H-HC-0.029500        0     0.3395   -5.34269  -6.46026  L
 H-HA-0.133000        0     1.42907  -4.53233  -4.03234  L
 H-HA-0.133000        0     2.07094  -2.68773  -7.87852  L
 H-HA-0.143000        0     3.53148  -3.49773  -3.20376  L
 H-HA-0.143000        0     4.16817  -1.67486  -7.04487  L
 H-HA-0.129700        0     4.86259  -2.01047  -4.70013  L
 N-N--0.254800        0    -1.03913  -1.61455  -4.48031  L
 C-CT--0.026600       0    -1.14454  -0.16664  -4.32397  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.18593   0.48491  -3.86799  H
 O-O--0.574800        0     0.60546   0.32212  -2.73212  H
 C-CT--0.007000       0    -2.22358  -0.00398  -3.25046  L
 C-CT-0.018900        0    -1.96854  -1.17677  -2.30163  L
 C-CT-0.019200        0    -1.31934  -2.24303  -3.18901  L
 H-H1-0.064100        0    -1.49323   0.29522  -5.23448  L
 H-HC-0.025300        0    -3.2091   -0.10361  -3.70445  L
 H-HC-0.025300        0    -2.14602   0.94787  -2.73135  L
 H-HC-0.021300        0    -2.89962  -1.53345  -1.86088  L
 H-HC-0.021300        0    -1.27587  -0.88126  -1.51567  L
 H-H1-0.039100        0    -0.39598  -2.59961  -2.73173  L
 H-H1-0.039100        0    -2.02068  -3.0634   -3.29654  L
 N-N--0.254800        0     0.8463    1.31705  -4.73635  H
 C-CT--0.026600       0     2.06412   1.95542  -4.26361  H
 C-C-0.589600         0     2.11427   3.4397   -4.64737  H
 O-O--0.574800        0     1.56346   3.87819  -5.64545  H
 C-CT--0.007000       0     3.14796   1.23004  -5.0775   H
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 C-CT-0.018900        0     2.50293   1.12977  -6.46749  H
 C-CT-0.019200        0     0.97743   1.10868  -6.19136  H
 H-H1-0.064100        0     2.16728   1.84296  -3.1847   H
 H-HC-0.025300        0     3.31855   0.24632  -4.63332  H
 H-HC-0.025300        0     4.0924    1.77782  -5.08549  H
 H-HC-0.021300        0     2.8321    0.25659  -7.02889  H
 H-HC-0.021300        0     2.74417   2.01788  -7.05471  H
 H-H1-0.039100        0     0.51259   1.93059  -6.72837  H
 H-H1-0.039100        0     0.51697   0.16637  -6.48345  H
 N-N--0.415700        0     2.94274   4.1117   -3.79337  H
 C-CT-0.039700        0     3.35729   5.50506  -3.93337  H
 C-C-0.597300         0     4.21462   5.63129  -5.23545  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.25089   4.96067  -5.31115  L
 C-CT--0.003600       0     4.0612    5.78035  -2.58053  H
 C-CT-0.013600        0     4.60377   7.16177  -2.29906  H
 C-C-0.805400         0     5.57383   7.18253  -1.11722  H
 O-O2--0.818800       0     6.10258   6.19579  -0.62058  H
 H-H-0.271900         0     2.84539   3.81803  -2.81919  H
 H-H1-0.110500        0     2.50186   6.18667  -4.02376  H
 H-HC--0.017300       0     3.3355    5.52498  -1.79988  H
 H-HC--0.017300       0     4.87949   5.09239  -2.39982  H
 H-HC--0.042500       0     3.79047   7.85984  -2.09135  H
 H-HC--0.042500       0     5.1552    7.57507  -3.14891  H
 N-N--0.254800        0     3.81629   6.38384  -6.2982   L
 C-CT--0.026600       -1    4.63879   6.63251  -7.50744  L
 C-C-0.589600         0     6.05782   7.15632  -7.2092   L
 O-O--0.574800        0     6.94465   7.02133  -8.05384  L
 C-CT--0.007000       0     3.83688   7.52336  -8.45266  L
 C-CT-0.018900        0     2.54396   7.85562  -7.71335  L
 C-CT-0.019200        0     2.49165   6.96715  -6.47038  L
 H-H1-0.064100        0     4.76435   5.67418  -8.00368  L
 H-HC-0.025300        0     3.60758   6.9705   -9.36449  L
 H-HC-0.025300        0     4.38267   8.43108  -8.7068   L
 H-HC-0.021300        0     1.69104   7.65494  -8.35992  L
 H-HC-0.021300        0     2.54876   8.90349  -7.41414  L
 H-H1-0.039100        0     2.20341   7.56611  -5.60684  L
 H-H1-0.039100        0     1.75726   6.17796  -6.62597  L
 N-N--0.415700        0     6.3217    7.68919  -6.0105   L
 C-CT-0.014300        -1    7.6695    7.86243  -5.47594  L
 C-C-0.597300         0     8.45879   6.55715  -5.45515  L
 O-O--0.567900        0     8.20081   5.63581  -4.67653  L
 C-CT--0.204100       0     7.64634   8.4764   -4.06449  L
 C-C-0.713000         0     9.03132   8.91895  -3.61406  L
 O-O--0.593100        0     9.73191   8.25878  -2.85855  L
 N-N--0.919100        0     9.5122    10.04031  -4.09182  L
 H-H-0.271900         0     5.51335   7.93118  -5.43519  L
 H-H1-0.104800        0     8.1821    8.56664  -6.13304  L
 H-HC-0.079700        0     7.30001   7.7334   -3.35056  L
 H-HC-0.079700        0     6.96461   9.32093  -4.04157  L
 H-H-0.419600         0     10.41636   10.30446  -3.75468  L
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H-H-0.419600          0     8.98006   10.6336  -4.72544  L
N-N--0.415700         0     9.5131    6.54023  -6.25534  L
C-CT--0.025200        -1    10.66723   5.72633  -5.96247  L
C-C-0.597300          0     11.00564   4.73583  -7.08293  L
O-O--0.567900         0     11.47366   5.10024  -8.15737  L
H-H-0.271900          0     9.58303   7.2567   -6.96238  L
H-H1-0.069800         0     10.53994   5.1859   -5.02374  L
H-H1-0.069800         0     11.52627   6.38553  -5.84094  L
N-N--0.415700         0     10.79216   3.46487  -6.77141  L
C-CT--0.001400        -1    10.80835   2.25113  -7.60051  L
C-C-0.597300          0     9.80296   1.32155  -6.90827  L
O-O--0.567900         0     9.07779   1.75456  -6.00376  L
C-CT--0.015200        0     12.2467   1.69119  -7.64709  L
C-CA--0.001100        0     12.7119   1.30647  -9.03655  L
C-CA--0.190600        0     13.1391   2.31605  -9.92117  L
C-CA--0.190600        0     12.73687  -0.04233  -9.44216  L
C-CA--0.234100        0     13.59951   1.98221  -11.20935  L
C-CA--0.234100        0     13.18733  -0.37941  -10.73327  L
C-C-0.322600          0     13.62187   0.63035  -11.61654  L
O-OH--0.557900        0     14.0521   0.30095  -12.86226  L
H-H-0.271900          0     10.32569   3.33234  -5.88443  L
H-H1-0.087600         0     10.45601   2.48315  -8.60706  L
H-HC-0.029500         0     12.34624   0.83769  -6.97535  L
H-HC-0.029500         0     12.94276   2.44688  -7.27851  L
H-HA-0.169900         0     13.10505   3.35209  -9.60518  L
H-HA-0.169900         0     12.41413  -0.82399  -8.76865  L
H-HA-0.165600         0     13.92333   2.76191  -11.88058  L
H-HA-0.165600         0     13.20478  -1.40761  -11.06074  L
H-HO-0.399200         0     14.32681   1.07762  -13.34938  L
N-N--0.415700         0     9.82083   0.0343   -7.20593  L
C-CT--0.051800        -1    9.3969   -0.9694   -6.23483  L
C-C-0.597300          0     10.55861  -1.89975  -5.93247  L
O-O--0.567900         0     11.51759  -2.01931  -6.69481  L
C-CT--0.110200        0     8.10874  -1.65907  -6.7333   L
C-CT-0.353100         0     8.19827  -2.41359  -8.07804  L
C-CT--0.412100        0     8.7275   -3.8422   -7.91354  L
C-CT--0.412100        0     6.80268  -2.51037  -8.69459  L
H-H-0.271900          0     10.37357  -0.259    -8.00116  L
H-H1-0.092200         0     9.16244  -0.47166  -5.29895  L
H-HC-0.045700         0     7.35666  -0.87358  -6.82625  L
H-HC-0.045700         0     7.74806  -2.34696  -5.96956  L
H-HC--0.036100        0     8.8377   -1.87353  -8.77505  L
H-HC-0.100000         0     9.76591  -3.82608  -7.59197  L
H-HC-0.100000         0     8.68137  -4.35795  -8.87275  L
H-HC-0.100000         0     8.12775  -4.38649  -7.18482  L
H-HC-0.100000         0     6.12979  -3.04929  -8.0332   L
H-HC-0.100000         0     6.8542   -3.01569  -9.65999  L
H-HC-0.100000         0     6.4075   -1.51087  -8.85371  L
N-N--0.415700         0     10.49174  -2.5177   -4.76656  L
C-CT--0.058100        -1    11.57655  -3.30558  -4.19838  L
C-C-0.597300          0     11.07942  -4.70013  -3.84139  L
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 O-O--0.567900        0     9.88295  -4.97993  -3.84676  L
 C-CT--0.007400       0     12.15094  -2.54047  -2.99216  L
 C-CC-0.186800        0     11.13238  -2.18683  -1.93021  L
 N-NB--0.543200       0     10.70972  -3.01943  -0.89375  L
 C-CW--0.220700       0     10.43425  -1.01694  -1.8673   L
 C-CR-0.163500        0     9.77325  -2.32676  -0.22267  L
 N-NA--0.279500       0     9.57597  -1.12889  -0.79456  L
 H-H-0.271900         0     9.6463   -2.38047  -4.22452  L
 H-H1-0.136000        0     12.36939  -3.42759  -4.9385   L
 H-HC-0.036700        0     12.59902  -1.61433  -3.35497  L
 H-HC-0.036700        0     12.94861  -3.12599  -2.54064  L
 H-H4-0.186200        0     10.50678  -0.19375  -2.56514  L
 H-H-0.333900         0     8.84372  -0.47913  -0.53395  L
 H-H5-0.143500        0     9.21673  -2.69179   0.63146  L
 N-N--0.415700        0     11.99398  -5.61221  -3.52937  L
 C-CT--0.059700       -1    11.60236  -6.98668  -3.21468  L
 C-C-0.597300         0     10.68251  -7.10886  -1.97413  L
 O-O--0.567900        0     9.92094  -8.06769  -1.8622   L
 C-CT-0.130300        0     12.83732  -7.8982   -3.11322  L
 C-CT--0.043000       0     12.37837  -9.36862  -3.02204  L
 C-CT--0.320400       0     13.76249  -7.51109  -1.94415  L
 C-CT--0.066000       -1    13.44246  -10.349   -3.49388  L
 H-H-0.271900         0     12.97065  -5.36492  -3.56003  L
 H-H1-0.086900        0     11.01999  -7.34414  -4.06157  L
 H-HC-0.018700        0     13.3994  -7.77699  -4.0414   L
 H-HC-0.023600        0     11.50635  -9.51929  -3.65925  L
 H-HC-0.023600        0     12.09917  -9.61361  -1.99639  L
 H-HC-0.088200        0     14.66483  -8.11854  -1.97579  L
 H-HC-0.088200        0     13.26446  -7.67184  -0.98734  L
 H-HC-0.088200        0     14.0641  -6.46739  -2.01837  L
 H-HC-0.018600        0     13.04775  -11.36384  -3.43734  L
 H-HC-0.018600        0     14.32699  -10.28139  -2.86093  L
 H-HC-0.018600        0     13.7173  -10.13395  -4.52712  L
 N-N--0.415700        0     10.69654  -6.13079  -1.06169  L
 C-CT--0.025200       -1    9.67505  -5.99456  -0.02237  L
 C-C-0.597300         0     8.2781   -5.87789  -0.62827  L
 O-O--0.567900        0     7.46141  -6.78972  -0.48365  L
 H-H-0.271900         0     11.31222  -5.34497  -1.21036  L
 H-H1-0.069800        0     9.88212  -5.1196    0.58947  L
 H-H1-0.069800        0     9.69598  -6.87486   0.61535  L
 N-N--0.415700        0     8.03124  -4.79367  -1.37423  L
 C-CT--0.058100       0     6.83528  -4.61905  -2.21233  L    H-HC
246   0.        0.
 C-C-0.597300         0     6.48898  -5.893    -3.00446  L
 O-O--0.567900        0     5.319    -6.26285  -3.06655  L
 C-CT--0.007400       0     7.01769  -3.4531   -3.18966  H
 C-CC-0.186800        0     6.96967  -2.02506  -2.73827  H
 N-NB--0.543200       0     7.65606  -1.1226   -3.51312  H
 C-CW--0.220700       0     6.20271  -1.35033  -1.82274  H
 C-CR-0.163500        0     7.25951   0.06458  -3.12075  H
 N-NA--0.279500       0     6.39233  -0.01062  -2.07673  H
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H-H-0.271900          0     8.79579  -4.1389   -1.49208  L
H-H1-0.136000         0     5.97622  -4.40263  -1.5743   L
H-HC-0.036700         0     6.24382  -3.57097  -3.95537  H
H-HC-0.036700         0     7.95504  -3.57712  -3.72499  H
H-H4-0.186200         0     5.53939  -1.65902  -1.0384   H
H-H-0.333900          0     5.80406   0.7566   -1.7376   H
H-H5-0.143500         0     7.593     1.01131  -3.53981  H
N-N--0.415700         0     7.48153  -6.59     -3.57529  L
C-CT-0.033700         -1    7.29184  -7.84794  -4.30474  L
C-C-0.597300          0     6.4884   -8.91481  -3.55663  L
O-O--0.567900         0     5.66305  -9.58701  -4.1744   L
C-CT--0.182500        0     8.60904  -8.37963  -4.87415  L
H-H-0.271900          0     8.40899  -6.18207  -3.53154  L
H-H1-0.082300         0     6.67972  -7.59312  -5.16798  L
H-HC-0.060300         0     9.15464  -7.57343  -5.36579  L
H-HC-0.060300         0     8.39192  -9.15315  -5.61204  L
H-HC-0.060300         0     9.21214  -8.82389  -4.08782  L
N-N--0.347900         0     6.65852  -9.05548  -2.23741  L
C-CT--0.240000        -1    5.7746   -9.91514  -1.43958  L
C-C-0.734100          0     4.29833  -9.46351  -1.49757  L
O-O--0.589400         0     3.42433  -10.31177  -1.65414  L
C-CT--0.009400        0     6.29113  -10.04503   0.00336  L
C-CT-0.018700         0     5.41314  -10.99888   0.83896  L
C-CT--0.047900        0     6.04204  -11.29286   2.20489  L
C-CT--0.014300        0     5.08169  -12.06689   3.11582  L
N-N3--0.385400        0     5.66715  -12.26815   4.46616  L
H-H-0.274700          0     7.33693  -8.44524  -1.78664  L
H-H1-0.142600         0     5.79142  -10.90972  -1.88883  L
H-HC-0.036200         0     6.30903  -9.06276   0.47665  L
H-HC-0.036200         0     7.31093  -10.43252  -0.02897  L
H-HC-0.010300         0     5.27878  -11.93904   0.30158  L
H-HC-0.010300         0     4.43611  -10.5402   0.99531  L
H-HC-0.062100         0     6.28548  -10.3424   2.67798  L
H-HC-0.062100         0     6.95458  -11.87266   2.05886  L
H-HP-0.113500         0     4.82738  -13.02515   2.65395  L
H-HP-0.113500         0     4.16179  -11.47932   3.20994  L
H-H-0.340000          0     4.94943  -12.52839   5.13859  L
H-H-0.340000          0     6.02211  -11.37661   4.81259  L
H-H-0.340000          0     6.4192   -12.93869   4.46721  L
N-N--0.415700         0     4.00993  -8.16244  -1.36824  L
C-CT--0.024900        -1    2.65754  -7.58813  -1.54406  L
C-C-0.597300          0     2.10399  -7.86213  -2.9529   L
O-O--0.567900         0     0.98075  -8.3497   -3.04966  L
C-CT-0.211700         0     2.63946  -6.08213  -1.22551  L
O-OH--0.654600        0     1.29923  -5.63786  -1.12928  L
H-H-0.271900          0     4.79759  -7.5289   -1.32762  L
H-H1-0.084300         0     1.98913  -8.07926  -0.83606  L
H-H1-0.035200         0     3.15617  -5.52186  -2.00395  L
H-H1-0.035200         0     3.13949  -5.91189  -0.27227  L
H-HO-0.427500         0     1.25688  -4.70571  -0.83932  L
N-N--0.415700         0     2.87761  -7.63301  -4.03163  L
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C-CT--0.059700       -1    2.54747  -8.06239  -5.41774  L
C-C-0.597300         0     2.13377  -9.55203  -5.39095  L
O-O--0.567900        0     1.00778  -9.87257  -5.75106  L
C-CT-0.130300        0     3.69824  -7.78442  -6.41579  L
C-CT--0.043000       0     4.07116  -6.28625  -6.42914  L
C-CT--0.320400       0     3.30332  -8.23438  -7.83501  L
C-CT--0.066000       0     5.30372  -5.94776  -7.27372  L
H-H-0.271900         0     3.77614  -7.194    -3.858    L
H-H1-0.086900        0     1.67589  -7.49506  -5.74651  L
H-HC-0.018700        0     4.57289  -8.3561   -6.11175  L
H-HC-0.023600        0     4.28081  -5.95371  -5.41519  L
H-HC-0.023600        0     3.22612  -5.71011  -6.80255  L
H-HC-0.088200        0     2.46831  -7.6364   -8.202    L
H-HC-0.088200        0     3.0198   -9.28689  -7.84911  L
H-HC-0.088200        0     4.14449  -8.11617  -8.51744  L
H-HC-0.018600        0     5.05502  -5.9738   -8.33472  L
H-HC-0.018600        0     6.11196  -6.64918  -7.07315  L
H-HC-0.018600        0     5.63684  -4.94573  -7.01318  L
N-N--0.415700        0     2.99708  -10.46092  -4.9185   L
C-CT-0.021300        -1    2.77454  -11.91982  -4.92406  L
C-C-0.597300         0     1.5541   -12.42386  -4.15501  L
O-O--0.567900        0     1.00593  -13.46345  -4.50641  L
C-CT--0.123100       -1    4.08476  -12.65671  -4.51107  L
S-SH--0.311900       0     5.42779  -12.31722  -5.68579  L
H-H-0.271900         0     3.9013   -10.12222  -4.61335  L
H-H1-0.112400        0     2.57527  -12.20308  -5.95953  L
H-H1-0.111200        0     3.89093  -13.7313  -4.50468  L
H-H1-0.111200        0     4.37879  -12.34607  -3.5077   L
H-HS-0.193300        0     5.58865  -11.02362  -5.36888  L
N-N--0.415700        0     1.12658  -11.71531  -3.11448  L
C-CT--0.051800       -1   -0.10563  -12.02462  -2.39532  L
C-C-0.597300         0    -1.33718  -11.38358  -3.06119  L
O-O--0.567900        0    -2.31256  -12.08906  -3.29317  L
C-CT--0.110200       0     0.04164  -11.54746  -0.93912  L
C-CT-0.353100        0     1.06123  -12.37101  -0.12811  L
C-CT--0.412100       0     1.40788  -11.63913   1.16639  L
C-CT--0.412100       0     0.52108  -13.75383   0.24373  L
H-H-0.271900         0     1.66634  -10.89817  -2.85714  L
H-H1-0.092200        0    -0.27602  -13.10195  -2.40091  L
H-HC-0.045700        0    -0.9292   -11.60623  -0.44468  L
H-HC-0.045700        0     0.34745  -10.49945  -0.94696  L
H-HC--0.036100       0     1.98221  -12.49747  -0.69634  L
H-HC-0.100000        0     1.85429  -10.67861   0.91304  L
H-HC-0.100000        0     2.11769  -12.2238   1.74673  L
H-HC-0.100000        0     0.5033   -11.46794   1.75188  L
H-HC-0.100000        0     1.25518  -14.29283   0.84024  L
H-HC-0.100000        0     0.32431  -14.33084  -0.6595   L
H-HC-0.100000        0    -0.40562  -13.65468   0.80988  L
N-N--0.415700        0    -1.31208  -10.08232  -3.39008  L
C-CT-0.014300        -1   -2.41299  -9.39055  -4.0895   L
C-C-0.597300         0    -2.77255  -10.07879  -5.39185  L
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O-O--0.567900        0    -3.92156  -10.47406  -5.59254  L
C-CT--0.204100       0    -2.1438   -7.88744  -4.19806  L
C-C-0.713000         0    -2.3528   -7.20302  -2.85498  L
O-O--0.593100        0    -3.46288  -6.89862  -2.44314  L
N-N--0.919100        0    -1.30334  -6.9407   -2.11681  L
H-H-0.271900         0    -0.45795  -9.56716  -3.21132  L
H-H1-0.104800        0    -3.30607  -9.50359  -3.46965  L
H-HC-0.079700        0    -2.86162  -7.45995  -4.89611  L
H-HC-0.079700        0    -1.1415   -7.6972   -4.57931  L
H-H-0.419600         0    -1.4356   -6.43651  -1.26055  L
H-H-0.419600         0    -0.38197  -7.21403  -2.43075  L
N-N--0.415700        0    -1.76059  -10.31047  -6.21619  L
C-CT--0.002400      -1    -1.90243  -11.13546  -7.39444  L
C-C-0.597300         0    -2.08586  -12.63041  -7.14652  L
O-O--0.567900        0    -2.56003  -13.34338  -8.02543  L
C-CT--0.034300       0    -0.76899  -10.84888  -8.39522  L
C-CA-0.011800        0    -0.90432  -9.49977  -9.08558  L
C-CA--0.125600       0    -1.63822  -9.4005   -10.28361  L
C-CA--0.125600       0    -0.35475  -8.33469  -8.51562  L
C-CA--0.170400       0    -1.83642  -8.14873  -10.89403  L
C-CA--0.170400       0    -0.54325  -7.08383  -9.1324   L
C-CA--0.107200       0    -1.29258  -6.98909  -10.31706  L
H-H-0.271900         0    -0.83641  -9.97351  -5.97263  L
H-H1-0.097800        0    -2.82439  -10.82999  -7.8925   L
H-HC-0.029500        0    -0.78627  -11.61837  -9.16849  L
H-HC-0.029500        0     0.19844  -10.92313  -7.90136  L
H-HA-0.133000        0    -2.08165  -10.28253  -10.72321  L
H-HA-0.133000        0     0.19111  -8.39376  -7.58957  L
H-HA-0.143000        0    -2.43293  -8.07028  -11.79356  L
H-HA-0.143000        0    -0.1361   -6.18811  -8.69036  L
H-HA-0.129700        0    -1.46774  -6.02569  -10.77712  L
N-N--0.415700        0    -1.75427  -13.09793  -5.94924  L
C-CT--0.025200      -1    -1.9622   -14.46927  -5.51612  L
C-C-0.597300         0    -3.42147  -14.88546  -5.36727  L
O-O--0.567900        0    -3.77398  -16.02251  -5.66662  L
H-H-0.271900         0    -1.39561  -12.44465  -5.2717   L
H-H1-0.069800        0    -1.47207  -14.61443  -4.55428  L
H-H1-0.069800        0    -1.49448  -15.14121  -6.23617  L
N-N--0.415700        0    -4.25746  -13.97419  -4.8719   L
C-CT--0.059700      -1    -5.7172   -14.13312  -4.8055   L
C-C-0.597300         0    -6.38183  -14.10035  -6.18513  L
O-O--0.567900        0    -7.39004  -14.77425  -6.39054  L
C-CT-0.130300        0    -6.27526  -13.08346  -3.7881   L
C-CT--0.043000       0    -5.94585  -13.56505  -2.33483  L
C-CT--0.320400      -1    -7.79145  -12.76333  -3.9398   L
C-CT--0.066000      -1    -5.26484  -12.55222  -1.38423  L
H-H-0.271900         0    -3.84672  -13.09216  -4.58969  L
H-H1-0.086900        0    -5.93903  -15.12671  -4.41405  L
H-HC-0.018700        0    -5.74333  -12.14709  -3.96471  L
H-HC-0.023600        0    -5.28313  -14.43021  -2.37845  L
H-HC-0.023600        0    -6.86455  -13.91226  -1.86026  L
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H-HC-0.088200        0    -7.97946  -12.29159  -4.90641  L
H-HC-0.088200        0    -8.10479  -12.07451  -3.15532  L
H-HC-0.088200        0    -8.37593  -13.68169  -3.87416  L
H-HC-0.018600        0    -4.31317  -12.23115  -1.79841  L
H-HC-0.018600        0    -5.0953   -13.01722  -0.41298  L
H-HC-0.018600        0    -5.91041  -11.68272  -1.25915  L
N-N--0.415700        0    -5.79447  -13.36525  -7.13258  L
C-CT--0.149000       -1   -6.19402  -13.37102  -8.52836  L
H-H-0.271900         0    -4.96317  -12.86047  -6.86802  L
H-H1-0.097600        0    -6.46501  -14.38335  -8.83376  L
H-H1-0.097600        0    -5.3701   -13.01731  -9.14935  L
H-H1-0.097600        0    -7.05828  -12.71631  -8.66106  L
C-CT--0.366200       -1   -8.63681  -10.24817  -10.70119  L
C-C-0.597200         0    -7.88378  -9.55956  -9.62934  L
O-O--0.567900        0    -8.23108  -9.58     -8.45622  L
H-HC-0.112300        0    -7.99778  -10.96926  -11.20518  L
H-HC-0.112300        0    -9.026    -9.50887  -11.39958  L
H-HC-0.112300        0    -9.47924  -10.766   -10.24106  L
N-N--0.415700        0    -6.82643  -8.93507  -10.0923  L
C-CT-0.021300        -1   -6.0358   -8.05606  -9.28978  L
C-C-0.597300         0    -5.54699  -6.9023   -10.16422  L
O-O--0.567900        0    -4.94834  -7.1581   -11.21278  L
C-CT--0.123100       0    -4.83121  -8.83525  -8.74005  L
S-SH--0.311900       0    -3.75688  -7.73495  -7.76104  L
H-H-0.271900         0    -6.64649  -8.95155  -11.08323  L
H-H1-0.112400        0    -6.62467  -7.66658  -8.46047  L
H-H1-0.111200        0    -4.26188  -9.25175  -9.57034  L
H-H1-0.111200        0    -5.18919  -9.65731  -8.11995  L
H-HS-0.193300        0    -3.28316  -7.02117  -8.79559  L
N-N--0.415700        0    -5.76533  -5.65548  -9.74347  L
C-CT-0.014300        -1   -5.31007  -4.49164  -10.49934  L
C-C-0.597300         0    -3.94117  -3.9339   -10.01738  L
O-O--0.567900        0    -3.3529   -4.39206  -9.0332   L
C-CT--0.204100       0    -6.44331  -3.45054  -10.6041  L
C-C-0.713000         0    -6.26483  -2.48138  -11.7718  L
O-O--0.593100        0    -5.42357  -2.66569  -12.64176  L
N-N--0.919100        0    -6.99717  -1.40381  -11.82638  L
H-H-0.271900         0    -6.28904  -5.52061  -8.88346  L
H-H1-0.104800        0    -5.12924  -4.82626  -11.52251  L
H-HC-0.079700        0    -6.5332   -2.88973  -9.67422  L
H-HC-0.079700        0    -7.37647  -3.98084  -10.78071  L
H-H-0.419600         0    -6.87368  -0.80043  -12.61022  L
H-H-0.419600         0    -7.79377  -1.27416  -11.18699  L
N-N--0.415700        0    -3.40431  -2.9344   -10.71808  L
C-CT--0.051800       -1   -2.25264  -2.11759  -10.33509  L
C-C-0.597300         0    -2.75377  -0.67002  -10.07975  L
O-O--0.567900        0    -3.17642  -0.00255  -11.02108  L
C-CT--0.110200       0    -1.19127  -2.17866  -11.452   L
C-CT-0.353100        0    -0.00502  -1.21131  -11.25705  L
C-CT--0.412100       0     0.8094   -1.54023  -10.00573  L
C-CT--0.412100       0     0.93854  -1.28946  -12.45808  L
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H-H-0.271900          0    -3.93532  -2.62509  -11.5291  L
H-H1-0.092200         0    -1.81661  -2.49742  -9.41067  L
H-HC-0.045700         0    -1.67751  -1.93031  -12.39735  L
H-HC-0.045700         0    -0.81652  -3.2003   -11.52523  L
H-HC--0.036100        0    -0.36623  -0.18649  -11.18156  L
H-HC-0.100000         0     1.15934  -2.57079  -10.05429  L
H-HC-0.100000         0     0.1956   -1.40195  -9.11623  L
H-HC-0.100000         0     1.6616   -0.86499  -9.93439  L
H-HC-0.100000         0     1.34483  -2.2965   -12.55199  L
H-HC-0.100000         0     1.75086  -0.5753   -12.32898  L
H-HC-0.100000         0     0.3889   -1.03518  -13.36459  L
N-N--0.347900         0    -2.71435  -0.17374  -8.8304   L
C-CT--0.263700        -1   -3.40475   1.06311  -8.37976  L
C-C-0.734100          0    -2.41806   2.08594  -7.85042  L
O-O--0.589400         0    -1.83895   1.8707   -6.79936  L
C-CT--0.000700        0    -4.42979   0.6689   -7.30909  L
C-CT-0.039000         0    -5.40121   1.80469  -6.96334  L
C-CT-0.048600         0    -6.1117    1.50711  -5.64116  L
N-N2--0.529500        0    -5.2668    1.84662  -4.48207  L
C-CA-0.807600         0    -5.6508    1.8636   -3.22499  L
N-N2--0.862700        0    -6.81033   1.45056  -2.83744  L
N-N2--0.862700        0    -4.87441   2.29575  -2.28813  L
H-H-0.274700          0    -2.25836  -0.73308  -8.1159   L
H-H1-0.156000         0    -3.94411   1.50537  -9.21955  L
H-HC-0.032700         0    -3.88996   0.3598   -6.41288  L
H-HC-0.032700         0    -5.01698  -0.17923  -7.6661   L
H-HC-0.028500         0    -6.14261   1.88749  -7.75946  L
H-HC-0.028500         0    -4.87512   2.757    -6.87716  L
H-H1-0.068700         0    -6.43069   0.46634  -5.6081   L
H-H1-0.068700         0    -7.01598   2.09741  -5.59529  L
H-H-0.345600          0    -4.36992   2.31861  -4.62686  L
H-H-0.447800          0    -7.05588   1.50539  -1.85895  L
H-H-0.447800          0    -7.32732   0.78666  -3.41267  L
H-H-0.447800          0    -5.16753   2.19537  -1.33069  L
H-H-0.447800          0    -3.95057   2.66332  -2.53815  L
N-N--0.415700         0    -2.19827   3.17636  -8.57185  L
C-CT--0.002400        -1   -1.30613   4.22688  -8.08808  L
C-C-0.597300          0    -1.9042    4.97581  -6.88409  L
O-O--0.567900         0    -3.07096   5.35732  -6.91404  L
C-CT--0.034300        0    -0.92035   5.16478  -9.23637  L
C-CA-0.011800         0     0.02846   4.49735  -10.2164  L
C-CA--0.125600        0     1.41451   4.51014  -9.96739  L
C-CA--0.125600        0    -0.47065   3.8055   -11.3367  L
C-CA--0.170400        0     2.29637   3.84675  -10.83967  L
C-CA--0.170400        0     0.4097    3.13095  -12.20191  L
C-CA--0.107200        0     1.79385   3.15292  -11.95505  L
H-H-0.271900          0    -2.73925   3.32818  -9.40505  L
H-H1-0.097800         0    -0.38682   3.75889  -7.73379  L
H-HC-0.029500         0    -0.4269    6.04499  -8.82064  L
H-HC-0.029500         0    -1.81895   5.50574  -9.75341  L
H-HA-0.133000         0     1.79744   5.02521  -9.09737  L
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 H-HA-0.133000        0    -1.53443   3.78066  -11.52701  L
 H-HA-0.143000        0     3.35721   3.87098  -10.64585  L
 H-HA-0.143000        0     0.01385   2.59596  -13.05367  L
 H-HA-0.129700        0     2.46646   2.63758  -12.62383  L
 N-N--0.516300        0    -1.09081   5.18977  -5.84306  L
 C-CT-0.038100        0    -1.46545   5.91143  -4.61931  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.67017   7.22814  -4.51286  L
 O-O--0.581900        0     0.2065    7.38738  -3.65382  L
 C-CT--0.030300       0    -1.27238   5.01509  -3.38581  H
 C-C-0.799400         0    -2.26204   3.87235  -3.23228  H
 O-O2--0.801400       0    -2.31668   3.35366  -1.99708  H
 O-O2--0.801400       0    -2.99751   3.39767  -4.06382  H
 H-H-0.293600         0    -0.16387   4.78285  -5.88212  L
 H-H1-0.088000        0    -2.52239   6.18206  -4.66485  L
 H-HC--0.012200       0    -1.37903   5.6335   -2.48704  H
 H-HC--0.012200       0    -0.25646   4.60156  -3.3756   H
 N-N--0.516300        0    -0.99568   8.16253  -5.4099   L
 C-CT-0.038100        0    -0.30803   9.42788  -5.72032  L
 C-C-0.536600         0    -0.85231   10.64604  -4.94826  L
 O-O--0.581900        0    -0.67859   11.79648  -5.35098  L
 C-CT--0.030300       0    -0.41033   9.66195  -7.24247  L
 C-C-0.799400         0    -1.81936   10.0051  -7.74736  L
 O-O2--0.801400       0    -2.7895    9.44696  -7.18389  L
 O-O2--0.801400       0    -1.90306   10.75219  -8.74819  L
 H-H-0.293600         0    -1.8008    8.00204  -6.01472  L
 H-H1-0.088000        0     0.74458   9.32841  -5.46299  L
 H-HC--0.012200       0    -0.09352   8.75831  -7.75807  L
 H-HC--0.012200       0     0.27831   10.46217  -7.52053  L
 N-N--0.415700        0    -1.48544   10.40162  -3.79925  L
 C-CT--0.038900       -1   -2.22961   11.37507  -2.97597  L
 C-C-0.597300         0    -1.34477   12.56032  -2.46399  L
 O-O--0.567900        0    -1.8966    13.53433  -1.95376  L
 C-CT-0.365400        0    -2.9209    10.67492  -1.81502  L
 O-OH--0.676100       0    -2.05925   9.80948  -1.10074  L
 C-CT--0.243800       -1   -4.02394   9.83803  -2.44171  L
 H-H-0.271900         0    -1.53006   9.43236  -3.52306  L
 H-H1-0.100700        0    -2.99408   11.83476  -3.60174  L
 H-H1-0.004300        0    -3.35418   11.40474  -1.13232  L
 H-HC-0.064200        0    -4.7117    10.48163  -2.98883  L
 H-HC-0.064200        0    -4.55649   9.34532  -1.63511  L
 H-HC-0.064200        0    -3.62025   9.07607  -3.10827  L
 H-HO-0.410200        0    -1.87237   10.2542  -0.23888  L
 N-N--0.415700        0    -0.00207   12.56099  -2.6422   L
 C-CT-0.014300        -1    0.9163    13.71948  -2.46129  L
 C-C-0.597300         0     1.88477   13.85979  -3.66378  L
 O-O--0.567900        0     3.05223   13.47985  -3.54253  L
 C-CT--0.204100       0     1.62441   13.62996  -1.09611  L
 C-C-0.713000         0     2.44851   14.8746  -0.79021  L
 O-O--0.593100        0     2.65624   15.76694  -1.60082  L
 N-N--0.919100        0     2.95534   14.9955   0.41187  L
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 H-H-0.271900         0     0.34311   11.77702  -3.18322  L
 H-H1-0.104800        0     0.30973   14.62348  -2.4227   L
 H-HC-0.079700        0     2.2793    12.76143  -1.0822   L
 H-HC-0.079700        0     0.87041   13.51338  -0.31613  L
 H-H-0.419600         0     3.46607   15.84377   0.55853  L
 H-H-0.419600         0     2.75099   14.33736   1.1523   L
 N-N--0.254800        0     1.46278   14.47669  -4.79302  L
 C-CT--0.026600       -1    2.20863   14.48783  -6.06514  L
 C-C-0.589600         0     3.57505   15.16158  -6.01996  L
 O-O--0.574800        0     4.38795   14.99503  -6.92623  L
 C-CT--0.007000       0     1.26471   15.0954  -7.10804  L
 C-CT-0.018900        0     0.26994   15.90144  -6.27756  L
 C-CT-0.019200        0     0.15897   15.09782  -4.98478  L
 H-H1-0.064100        0     2.38464   13.45012  -6.35083  L
 H-HC-0.025300        0     0.73468   14.29074  -7.62139  L
 H-HC-0.025300        0     1.78852   15.72198  -7.83111  L
 H-HC-0.021300        0    -0.69438   15.994   -6.77821  L
 H-HC-0.021300        0     0.688     16.88533  -6.06006  L
 H-H1-0.039100        0    -0.09922   15.76316  -4.16095  L
 H-H1-0.039100        0    -0.60246   14.32466  -5.09539  L
 N-N--0.415700        0     3.88075   15.90672  -4.96136  L
 C-CT--0.025200       -1    5.04862   16.77246  -4.92053  L
 C-C-0.597300         0     6.40264   16.13722  -4.62124  L
 O-O--0.567900        0     7.35746   16.82024  -4.25718  L
 H-H-0.271900         0     3.23609   15.89873  -4.18041  L
 H-H1-0.069800        0     4.87752   17.53194  -4.15801  L
 H-H1-0.069800        0     5.13772   17.28995  -5.87621  L
 N-N--0.347900        0     6.47952   14.83076  -4.8191   L
 C-CT--0.240000       -1    7.64708   13.95115  -4.72666  L
 C-C-0.734100         0     7.55938   12.87427  -5.8427   L
 O-O--0.589400        0     8.34089   11.9231  -5.82259  L
 C-CT--0.009400       0     7.65745   13.34262  -3.293    L
 C-CT-0.018700        0     6.50033   12.34184  -3.17378  L    H-HC
590   0.        0.
 C-CT--0.047900       0     5.98975   11.79619  -1.84014  H
 C-CT--0.014300       0     4.76935   10.99755  -2.30922  H
 N-N3--0.385400       0     4.1026    10.17278  -1.29825  H
 H-H-0.274700         0     5.59285   14.42097  -5.0884   L
 H-H1-0.142600        0     8.55771   14.53008  -4.88235  L
 H-HC-0.036200        0     7.53842   14.13705  -2.55411  L
 H-HC-0.036200        0     8.60191   12.82894  -3.10981  L
 H-HC-0.010300        0     6.80542   11.47501  -3.74717  L
 H-HC-0.010300        0     5.63822   12.80347  -3.64565  L
 H-HC-0.062100        0     5.706     12.61604  -1.17849  H
 H-HC-0.062100        0     6.74419   11.16452  -1.37009  H
 H-HP-0.113500        0     5.06686   10.2947  -3.09645  H
 H-HP-0.113500        0     4.0416    11.67455  -2.77283  H
 H-H-0.340000         0     3.20983   9.88079  -1.69987  H
 H-H-0.340000         0     3.90348   10.70796  -0.45014  H
 H-H-0.340000         0     5.17223   9.07307  -0.93669  H
 N-N--0.516300        0     6.58245   12.96161  -6.76282  L
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C-CT-0.039700        -1    6.0874    11.84964  -7.6033   L
C-C-0.536600         0     6.26768   12.15738  -9.11807  L
O-O--0.581900        0     6.05665   13.28552  -9.55537  L
C-CT-0.056000        0     4.65623   11.3994   -7.21485  L
C-CT-0.013600        0     4.56638   11.26155  -5.68855  L
C-C-0.805400         0     3.65642   10.1877   -5.08654  L
O-O2--0.818800       0     2.6406    10.5258   -4.44488  L
O-O2--0.818800       0     4.14528   9.03864   -5.02822  L
H-H-0.293600         0     6.02755   13.80901  -6.82257  L
H-H1-0.110500        0     6.72316   10.98671  -7.40531  L
H-HC--0.017300       0     4.45939   10.43774  -7.68237  L
H-HC--0.017300       0     3.92043   12.12321  -7.56497  L
H-HC--0.042500       0     4.32073   12.23955  -5.28477  L
H-HC--0.042500       0     5.56104   10.98894  -5.34861  L
N-N--0.415700        0     6.73629   11.18226  -9.92443  L
C-CT--0.149000       -1    7.11861   11.35828  -11.34376  L
H-H-0.271900         0     6.86991   10.27448  -9.50595  L
H-H1-0.097600        0     7.89707   12.11923  -11.42037  L
H-H1-0.097600        0     6.24873   11.69307  -11.91256  L
H-H1-0.097600        0     7.48234   10.41717  -11.75696  L
C-CT--0.366200       0     10.20265   1.71353  -12.18899  L
C-C-0.597200         0     9.09662   1.08348   -11.3778  L
O-O--0.567900        0     9.33426   0.67012   -10.24751  L
H-HC-0.112300        0     10.76245   2.38248  -11.53814  L
H-HC-0.112300        0     9.79879   2.27831   -13.02625  L
H-HC-0.112300        0     10.86033   0.92429  -12.54776  L
N-N--0.415700        0     7.89165   1.02903   -11.95326  L
C-CT--0.059700       -1    6.69719   0.42512   -11.33914  L
C-C-0.597300         0     5.95217  -0.4665    -12.35044  L
O-O--0.567900        0     6.18393  -1.67121   -12.37201  L
C-CT-0.130300        0     5.80138   1.47983   -10.62368  L
C-CT--0.043000       0     6.59592   2.22815   -9.52136  L
C-CT--0.320400       0     4.55505   0.81938   -9.9935   L
C-CT--0.066000       0     5.83143   3.35022   -8.81066  L
H-H-0.271900         0     7.82648   1.37959   -12.89414  L
H-H1-0.086900        0     7.04417  -0.25909   -10.56562  L
H-HC-0.018700        0     5.46705   2.21013   -11.36251  L
H-HC-0.023600        0     7.46992   2.69976   -9.96753  L
H-HC-0.023600        0     6.94351   1.51239   -8.77435  L
H-HC-0.088200        0     3.99357   0.23987   -10.72446  L
H-HC-0.088200        0     3.87681   1.5795    -9.60616  L
H-HC-0.088200        0     4.84748   0.16423   -9.17372  L
H-HC-0.018600        0     5.01425   2.94727   -8.21283  L
H-HC-0.018600        0     5.44189   4.05254   -9.54712  L
H-HC-0.018600        0     6.5137    3.88278   -8.14705  L
N-N--0.415700        0     5.07314   0.09933   -13.19133  L
C-CT--0.149000       -1    4.25187  -0.64973   -14.14799  L
H-H-0.271900         0     4.92611   1.09194   -13.10169  L
H-H1-0.097600        0     3.79299  -1.50673   -13.6496  L
H-H1-0.097600        0     4.87685  -1.01794   -14.96335  L
H-H1-0.097600        0     3.46466  -0.01231   -14.5536  L
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C-CT--0.366200       -1   -5.09096   16.94807  -3.21789  L
C-C-0.597200         0    -5.66352   16.18587  -2.036    L
O-O--0.567900        0    -5.50966   16.642    -0.90609  L
H-HC-0.112300        0    -5.90025   17.34434  -3.82602  L
H-HC-0.112300        0    -4.46119   16.27867  -3.80269  L
H-HC-0.112300        0    -4.48087   17.76697  -2.84106  L
N-N--0.254800        0    -6.38372   15.07785  -2.2751   L
C-CT--0.026600       -1   -7.06765   14.32904  -1.22704  L
C-C-0.589600         0    -6.2109    13.22781  -0.60449  L
O-O--0.574800        0    -5.68537   12.34345  -1.27769  L
C-CT--0.007000       0    -8.27477   13.71857  -1.94918  L
C-CT-0.018900        0    -7.7449    13.4317   -3.35706  L
C-CT-0.019200        0    -6.74885   14.56838  -3.59309  L
H-H1-0.064100        0    -7.4229    15.00404  -0.44779  L
H-HC-0.025300        0    -9.07386   14.45903  -2.00745  L
H-HC-0.025300        0    -8.63695   12.81413  -1.46057  L
H-HC-0.021300        0    -8.54608   13.43934  -4.09641  L
H-HC-0.021300        0    -7.22345   12.47449  -3.37896  L
H-H1-0.039100        0    -5.87123   14.1936   -4.12235  L
H-H1-0.039100        0    -7.23088   15.35627  -4.17258  L
N-N--0.415700        0    -6.14437   13.27336   0.71847  L
C-CT--0.023700       -1   -5.28616   12.4455    1.55324  L
C-C-0.597300         0    -5.47093   10.91674   1.44018  L
O-O--0.567900        0    -6.56294   10.43001   1.13346  L
C-CT-0.034200        0    -5.53202   12.82595   3.02735  L
C-CT-0.001800        0    -5.09833   14.24934   3.40818  L
S-S--0.273700        0    -3.3152    14.51771   3.61689  L
C-CT--0.053600       -1   -3.00036   13.55372   5.12427  L
H-H-0.271900         0    -6.61791   14.04189   1.15984  L
H-H1-0.088000        0    -4.24526   12.66623   1.30436  L
H-HC-0.024100        0    -5.01218   12.1222    3.67742  L
H-HC-0.024100        0    -6.5988    12.72497   3.23402  L
H-H1-0.044000        0    -5.58024   14.506     4.35168  L
H-H1-0.044000        0    -5.46366   14.94806   2.65572  L
H-H1-0.068400        0    -3.16875   12.49373   4.92987  L
H-H1-0.068400        0    -3.65681   13.88839   5.92658  L
H-H1-0.068400        0    -1.96112   13.68358   5.42584  L
N-N--0.415700        0    -4.41101   10.16987   1.78671  L
C-CT--0.001400       -1   -4.28056   8.71771    1.62827  L
C-C-0.597300         0    -5.51174   7.83753    1.94426  L
O-O--0.567900        0    -6.10783   7.32805    1.00044  L
C-CT--0.015200       0    -2.98512   8.16657    2.24061  L
C-CA--0.001100       0    -2.90848   6.65747    2.39755  L
C-CA--0.190600       0    -3.04077   5.78893    1.29333  L
C-CA--0.190600       0    -2.77762   6.12604    3.689    L
C-CA--0.234100       0    -3.08554   4.39215    1.50066  L
C-CA--0.234100       0    -2.84913   4.74273    3.90234  L
C-C-0.322600         0    -3.01916   3.87215    2.81315  L
O-OH--0.557900       0    -3.14357   2.54036    3.03834  L
H-H-0.271900         0    -3.53762   10.65946   1.96498  L
H-H1-0.087600        0    -4.1457    8.57815    0.55559  L
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H-HC-0.029500        0    -2.85187   8.62731   3.21811  L
H-HC-0.029500        0    -2.15808   8.45212   1.59796  L
H-HA-0.169900        0    -3.18292   6.20404   0.30267  L
H-HA-0.169900        0    -2.69505   6.78983   4.53641  L
H-HA-0.165600        0    -3.25256   3.71443   0.67459  L
H-HA-0.165600        0    -2.83992   4.36405   4.91232  L
H-HO-0.399200        0    -3.47638   2.39335   3.94435  L
N-N--0.516300        0    -5.86498   7.55274   3.20546  L
C-CT-0.038100        -1   -6.82103   6.47856   3.57599  L
C-C-0.536600         0    -8.22739   6.69586   3.01372  L
O-O--0.581900        0    -8.893     5.73293   2.63992  L
C-CT--0.030300       0    -6.87405   6.2945    5.10554  L
C-C-0.799400         0    -5.60955   5.6361    5.67638  L
O-O2--0.801400       0    -5.50657   4.38815   5.58221  L
O-O2--0.801400       0    -4.7414    6.37165   6.20998  L
H-H-0.293600         0    -5.36852   8.0359    3.94962  L
H-H1-0.088000        0    -6.4518    5.54092   3.16553  L
H-HC--0.012200       0    -7.72192   5.65327   5.349    L
H-HC--0.012200       0    -7.05209   7.25689   5.58692  L
N-N--0.415700        0    -8.66609   7.95337   2.91672  L
C-CT--0.002400       0    -9.86161   8.34451   2.16844  L
C-C-0.597300         0    -9.77086   7.89008   0.70328  L
O-O--0.567900        0    -10.62847   7.14955   0.22179  L
C-CT--0.034300       0    -10.06118   9.86379   2.28128  L
C-CA-0.011800        0    -11.1189   10.40826   1.33919  L
C-CA--0.125600       0    -12.4851   10.24672   1.63647  L
C-CA--0.125600       0    -10.73492   11.02086   0.13062  L
C-CA--0.170400       0    -13.46211   10.70024   0.73144  L
C-CA--0.170400       0    -11.71087   11.47172  -0.77504  L
C-CA--0.107200       0    -13.0751   11.31218  -0.4744   L
H-H-0.271900         0    -8.01046   8.66521   3.20621  L
H-H1-0.097800        0    -10.72884   7.84711   2.60408  L
H-HC-0.029500        0    -9.11601   10.36603   2.06962  L
H-HC-0.029500        0    -10.33837   10.10798   3.30748  L
H-HA-0.133000        0    -12.78414   9.75496   2.55102  L
H-HA-0.133000        0    -9.68634   11.11801  -0.11843  L
H-HA-0.143000        0    -14.50979   10.56139   0.9556   L
H-HA-0.143000        0    -11.4061   11.92104  -1.70961  L
H-HA-0.129700        0    -13.82467   11.64614  -1.17739  L
N-N--0.415700        0    -8.73652   8.32518  -0.01375  L
C-CT--0.038900       -1   -8.55385   8.01541  -1.43611  L
C-C-0.597300         0    -8.38873   6.53271  -1.71521  L
O-O--0.567900        0    -9.0491    5.97606  -2.59013  L
C-CT-0.365400        0    -7.40014   8.83835  -2.02002  L
O-OH--0.676100       0    -7.65455   10.20926  -1.79372  L
C-CT--0.243800       0    -7.25952   8.65909  -3.53219  L
H-H-0.271900         0    -8.05379   8.93446   0.42674  L
H-H1-0.100700        0    -9.45856   8.32822  -1.95693  L
H-H1-0.004300        0    -6.47928   8.54697  -1.52113  L
H-HC-0.064200        0    -8.20918   8.8766   -4.0211   L
H-HC-0.064200        0    -6.95663   7.63858  -3.76534  L
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H-HC-0.064200        0    -6.50322   9.3395   -3.92063  L
H-HO-0.410200        0    -6.80847   10.65772  -1.63526  L
N-N--0.415700        0    -7.53781   5.88934  -0.92695  L
C-CT--0.058100       -1   -7.39278   4.44809  -0.7991   L
C-C-0.597300         0    -8.73609   3.74877  -0.6492   L
O-O--0.567900        0    -9.04661   2.88006  -1.46328  L
C-CT--0.007400       0    -6.43525   4.20784   0.37083  L
C-CC-0.186800        0    -6.34618   2.79232   0.84866  L
N-NB--0.543200       0    -6.48067   1.66269   0.04977  L
C-CW--0.220700       0    -6.20841   2.41453   2.14719  L
C-CR-0.163500        0    -6.45714   0.6153    0.88037  L
N-NA--0.279500       0    -6.27594   1.04253   2.14017  L
H-H-0.271900         0    -7.06113   6.46661  -0.24059  L
H-H1-0.136000        0    -6.93937   4.05914  -1.71012  L
H-HC-0.036700        0    -6.76969   4.8064    1.21155  L
H-HC-0.036700        0    -5.44299   4.54914   0.08211  L
H-H4-0.186200        0    -6.10936   3.06577   3.00788  L
H-H-0.333900         0    -6.25527   0.43411   2.95594  L
H-H5-0.143500        0    -6.59285  -0.41576   0.57667  L
N-N--0.415700        0    -9.53871   4.13141   0.34899  L
C-CT-0.021300        -1   -10.83442   3.5015    0.55697  L
C-C-0.597300         0    -11.75056   3.54453  -0.6437   L
O-O--0.567900        0    -12.37109   2.54359  -0.99896  L
C-CT--0.123100       0    -11.48893   3.89414   1.8988   L
S-SH--0.311900       0    -12.57425   5.34782   1.8219   L
H-H-0.271900         0    -9.23659   4.85632   0.9921   L
H-H1-0.112400        0    -10.61     2.43883   0.6627   L
H-H1-0.111200        0    -10.71608   4.05855   2.64912  L
H-H1-0.111200        0    -12.09197   3.05066   2.23848  L
H-HS-0.193300        0    -11.66286   6.18579   1.3085   L
N-N--0.415700        0    -11.78912   4.70266  -1.28161  L
C-CT--0.059700       -1   -12.61567   4.921    -2.44094  L
C-C-0.597300         0    -12.14782   4.19111  -3.7009   L
O-O--0.567900        0    -12.96616   3.56795  -4.37364  L
C-CT-0.130300        0    -12.8466   6.44534  -2.62517  L
C-CT--0.043000       0    -14.18144   6.89124  -1.97716  L
C-CT--0.320400       -1   -12.75903   6.94663  -4.07123  L
C-CT--0.066000       -1   -15.47271   6.48309  -2.71792  L
H-H-0.271900         0    -11.24069   5.46595  -0.89992  L
H-H1-0.086900        0    -13.58463   4.47505  -2.21888  L
H-HC-0.018700        0    -12.05274   6.97161  -2.09124  L
H-HC-0.023600        0    -14.17393   7.97886  -1.89281  L
H-HC-0.023600        0    -14.22321   6.49204  -0.9625   L
H-HC-0.088200        0    -11.74132   6.83024  -4.44556  L
H-HC-0.088200        0    -13.00804   8.00717  -4.10865  L
H-HC-0.088200        0    -13.44451   6.39458  -4.7158   L
H-HC-0.018600        0    -16.3362   6.7915   -2.12834  L
H-HC-0.018600        0    -15.50883   5.40243  -2.85503  L
H-HC-0.018600        0    -15.52332   6.97321  -3.68999  L
N-N--0.415700        0    -10.86041   4.27249  -4.03246  L
C-CT--0.024900       -1   -10.25904   3.56828  -5.17043  L
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C-C-0.597300          0    -10.47263   2.04632  -5.00715  L
O-O--0.567900         0    -10.94649   1.40338  -5.93753  L
C-CT-0.211700         0    -8.80145    4.01632  -5.28339  L
O-OH--0.654600        0    -8.31961    3.83119  -6.59767  L
H-H-0.271900          0    -10.25985    4.81487  -3.41963  L
H-H1-0.084300         0    -10.77857    3.8762   -6.07823  L
H-H1-0.035200         0    -8.18849    3.48767  -4.55322  L
H-H1-0.035200         0    -8.74652    5.08389  -5.06502  L
H-HO-0.427500         0    -7.54761    4.39151  -6.72592  L
N-N--0.516300         0    -10.25313    1.47306  -3.80949  L
C-CT-0.038100         -1   -10.56232    0.05686  -3.50891  L
C-C-0.536600          0    -12.04426  -0.32624  -3.64397  L
O-O--0.581900         0    -12.3783  -1.28348  -4.34867  L
C-CT--0.030300        0    -10.02199  -0.37255  -2.12714  L
C-C-0.799400          0    -8.61123  -0.95524  -2.20719  L
O-O2--0.801400        0    -7.99237  -0.88484  -3.29002  L
O-O2--0.801400        0    -8.0955   -1.4703   -1.19011  L
H-H-0.293600          0    -9.90332    2.05622  -3.05642  L
H-H1-0.088000         0    -10.07098  -0.53724  -4.27625  L
H-HC--0.012200        0    -10.67015  -1.14544  -1.71157  L
H-HC--0.012200        0    -10.04149    0.46941  -1.43536  L
N-N--0.415700         0    -12.93114    0.39724  -2.95696  L
C-CT-0.033700         -1   -14.38438    0.25137  -3.05559  L
C-C-0.597300          0    -14.87331    0.26168  -4.51626  L
O-O--0.567900         0    -15.71381  -0.55043  -4.89923  L
C-CT--0.182500        -1   -14.99587    1.41335  -2.33277  L
H-H-0.271900          0    -12.57531    1.15875  -2.38797  L
H-H1-0.082300         0    -14.69509  -0.68561  -2.5928   L
H-HC-0.060300         0    -14.72204    1.37598  -1.27799  L
H-HC-0.060300         0    -16.08276    1.35728  -2.40633  L
H-HC-0.060300         0    -14.66007    2.35915  -2.75687  L
N-N--0.415700         0    -14.37952    1.22674  -5.29867  L
C-CT--0.025200        -1   -14.7478    1.47529  -6.68751  L
C-C-0.597300          0    -14.25843    0.40673  -7.661    L
O-O--0.567900         0    -15.00549  -0.01215  -8.54059  L
H-H-0.271900          0    -13.70473    1.85829  -4.87836  L
H-H1-0.069800         0    -14.32976    2.43182  -6.9988   L
H-H1-0.069800         0    -15.83344    1.53014  -6.76445  L
N-N--0.516300         0    -13.00306  -0.01022  -7.51148  L
C-CT-0.039700         -1   -12.3706  -1.10387  -8.25332  L
C-C-0.536600          0    -13.10135  -2.44801  -8.07413  L
O-O--0.581900         0    -13.24336  -3.20927  -9.02821  L
C-CT-0.056000         0    -10.90267  -1.16317  -7.79859  L
C-CT-0.013600         0    -10.03097  -2.25429  -8.43084  L
C-C-0.805400          0    -9.59942  -1.97241  -9.87252  L
O-O2--0.818800        0    -9.59734  -2.92046  -10.68979  L
O-O2--0.818800        0    -9.10293  -0.85767  -10.14165  L
H-H-0.293600          0    -12.43236    0.44554  -6.80459  L
H-H1-0.110500         0    -12.38937  -0.86997  -9.31856  L
H-HC--0.017300        0    -10.90402  -1.32222  -6.72258  L
H-HC--0.017300        0    -10.43438  -0.19576  -7.98093  L
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H-HC--0.042500       0    -10.55747  -3.20268  -8.36733  L
H-HC--0.042500       0    -9.12156  -2.34642  -7.83418  L
N-N--0.415700        0    -13.55172  -2.74982  -6.85149  L
C-CT--0.025200       -1   -14.25385  -3.99318  -6.49736  L
C-C-0.597300         0    -13.50734  -4.84718  -5.48801  L
O-O--0.567900        0    -13.85021  -6.02046  -5.32262  L
H-H-0.271900         0    -13.42337  -2.03471  -6.14423  L
H-H1-0.069800        0    -14.42432  -4.59748  -7.38873  L
H-H1-0.069800        0    -15.22312  -3.73698  -6.07154  L
N-N--0.415700        0    -12.49596  -4.28451  -4.80985  L
C-CT--0.059700       -1   -11.75828  -4.98727  -3.75953  L
C-C-0.597300         0    -12.77303  -5.52357  -2.74509  L
O-O--0.567900        0    -13.70105  -4.82274  -2.34699  L
C-CT-0.130300        0    -10.67953  -4.09219  -3.09496  L
C-CT--0.043000       0    -9.37299  -4.08339  -3.90633  L
C-CT--0.320400       0    -10.25914  -4.57692  -1.6904   L
C-CT--0.066000       0    -9.44411  -3.45988  -5.29431  L
H-H-0.271900         0    -12.33763  -3.29164  -4.94583  L
H-H1-0.086900        0    -11.26821  -5.83576  -4.2191   L
H-HC-0.018700        0    -11.06043  -3.07771  -2.99741  L
H-HC-0.023600        0    -9.04703  -5.10717  -4.01701  L
H-HC-0.023600        0    -8.61088  -3.54814  -3.34398  L
H-HC-0.088200        0    -9.49415  -3.91318  -1.28322  L
H-HC-0.088200        0    -9.86374  -5.59214  -1.73965  L
H-HC-0.088200        0    -11.10334  -4.54359  -1.00953  L
H-HC-0.018600        0    -8.45491  -3.47996  -5.7492   L
H-HC-0.018600        0    -9.76973  -2.42934  -5.20675  L
H-HC-0.018600        0    -10.13136  -4.01471  -5.92872  L
N-N--0.415700        0    -12.59009  -6.77562  -2.3232   L
C-CT--0.025200       -1   -13.44456  -7.41949  -1.31747  L
C-C-0.597300         0    -12.89098  -7.35139   0.08894  L
O-O--0.567900        0    -13.61897  -7.15144   1.05927  L
H-H-0.271900         0    -11.84745  -7.2832   -2.78696  L
H-H1-0.069800        0    -13.57454  -8.46775  -1.58163  L
H-H1-0.069800        0    -14.43153  -6.95426  -1.31719  L
N-N--0.415700        0    -11.58178  -7.53919   0.181    L
C-CT--0.058100       -1   -10.82713  -7.52688   1.41558  L
C-C-0.597300         0    -9.45013  -6.88412   1.14496  L
O-O--0.567900        0    -8.71251  -7.3752    0.29139  L
C-CT--0.007400       0    -10.67679  -8.96917   1.93015  L
C-CC-0.186800        0    -11.97268  -9.55754   2.44051  L
N-NB--0.543200       0    -12.57077  -9.27829   3.67264  L
C-CW--0.220700       0    -12.79025  -10.38705   1.73012  L
C-CR-0.163500        0    -13.74107  -9.93114   3.66889  L
N-NA--0.279500       0    -13.89881  -10.60977   2.51846  L
H-H-0.271900         0    -11.0609  -7.65425  -0.67666  L
H-H1-0.136000        0    -11.34662  -6.93716   2.17251  L
H-HC-0.036700        0    -9.93982  -8.99199   2.73045  L
H-HC-0.036700        0    -10.29218  -9.59929   1.12671  L
H-H4-0.186200        0    -12.60704  -10.74621   0.72766  L
H-H-0.333900         0    -14.71675  -11.14496   2.26786  L
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H-H5-0.143500        0    -14.46019  -9.90149   4.47735  L
N-N--0.415700        0    -9.10273   -5.77637   1.8129   L
C-CT--0.024900       -1   -7.84258   -5.04319   1.57677  L
C-C-0.597300         0    -6.64954   -5.66976   2.29956  L
O-O--0.567900        0    -6.69348   -5.94799   3.49781  L
C-CT-0.211700        0    -7.97078   -3.54876   1.8988   L
O-OH--0.654600       0    -6.69245   -2.92561   1.8649   L
H-H-0.271900         0    -9.71843   -5.4762    2.56068  L
H-H1-0.084300        0    -7.63243   -5.09489   0.50771  L
H-H1-0.035200        0    -8.41463   -3.42836   2.88033  L
H-H1-0.035200        0    -8.62599   -3.07439   1.16571  L
H-HO-0.427500        0    -6.71237   -2.15144   2.45906  L
N-N--0.415700        0    -5.55513   -5.85907   1.55986  L
C-CT--0.051800       -1   -4.25482   -6.2655    2.08747  L
C-C-0.597300         0    -3.35912   -5.05863   2.30183  L
O-O--0.567900        0    -3.12004   -4.30031   1.36395  L
C-CT--0.110200       0    -3.5842    -7.26616   1.12184  L
C-CT-0.353100        0    -4.0998    -8.71743   1.1705   L
C-CT--0.412100       0    -5.49481   -8.896     0.57065  L
C-CT--0.412100       0    -3.1409    -9.61063   0.37639  L
H-H-0.271900         0    -5.63354   -5.64523   0.57734  L
H-H1-0.092200        0    -4.3914    -6.76053   3.05208  L
H-HC-0.045700        0    -2.52672   -7.298     1.37432  L
H-HC-0.045700        0    -3.65762   -6.894     0.10315  L
H-HC--0.036100       0    -4.10899   -9.06022   2.20544  L
H-HC-0.100000        0    -5.52767   -8.49271  -0.44211  L
H-HC-0.100000        0    -6.23619   -8.38718   1.18446  L
H-HC-0.100000        0    -5.75779   -9.95245   0.54454  L
H-HC-0.100000        0    -2.13796   -9.54354   0.79706  L
H-HC-0.100000        0    -3.11894   -9.29535  -0.66751  L
H-HC-0.100000        0    -3.47492   -10.64661   0.42872  L
N-N--0.415700        0    -2.82468   -4.92256   3.50793  L
C-CT-0.021300        -1   -1.88546   -3.86184   3.84062  L
C-C-0.597300         0    -0.74798   -4.37281   4.74286  L
O-O--0.567900        0    -0.75106   -5.53141   5.16228  L
C-CT--0.123100       0    -2.69614   -2.72375   4.4707   L
S-SH--0.311900       0    -1.7546    -1.17656   4.4897   L
H-H-0.271900         0    -3.09231   -5.57075   4.24084  L
H-H1-0.112400        0    -1.42202   -3.47972   2.92737  L
H-H1-0.111200        0    -2.99607   -2.99271   5.48513  L
H-H1-0.111200        0    -3.59222   -2.55825   3.87157  L
H-HS-0.193300        0    -2.68202   -0.45453   5.13429  L
N-N--0.415700        0     0.23816   -3.5351    5.06322  L
C-CT--0.038900       -1    1.35021   -3.90158   5.95269  L
C-C-0.597300         0     1.47364   -3.00235   7.15945  L
O-O--0.567900        0     0.80501   -1.98531   7.31786  L
C-CT-0.365400        0     2.70414   -4.02846   5.22642  L
O-OH--0.676100       0     3.10145   -2.83418   4.58903  L
C-CT--0.243800       0     2.70172   -5.17495   4.2187   L
H-H-0.271900         0     0.14794   -2.57786   4.7429   L
H-H1-0.100700        0     1.14216   -4.88834   6.36623  L
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H-H1-0.004300        0     3.47349  -4.27448   5.95829  L
H-HC-0.064200        0     1.98004  -4.99042   3.42494  L
H-HC-0.064200        0     2.43389  -6.10526   4.72055  L
H-HC-0.064200        0     3.69387  -5.27703   3.78846  L
H-HO-0.410200        0     3.44639  -2.22218   5.27984  L
N-N--0.415700        0     2.31753  -3.47877   8.0653   L
C-CT--0.051800       -1    2.23479  -3.17486   9.47098  L
C-C-0.597300         0     2.32741  -1.67475   9.84637  L
O-O--0.567900        0     1.78895  -1.28443   10.87318  L
C-CT--0.110200       0     3.24005  -4.044     10.19541  L
C-CT-0.353100        0     2.94208  -4.11649   11.69461  L
C-CT--0.412100       0     1.60599  -4.77298   12.05346  L
C-CT--0.412100       -1    4.04364  -4.9988    12.21931  L
H-H-0.271900         0     2.77743  -4.33673   7.81852  L
H-H1-0.092200        0     1.23278  -3.47939   9.77457  L
H-HC-0.045700        0     4.23693  -3.63174   10.03087  L
H-HC-0.045700        0     3.19946  -5.05398   9.78226  L
H-HC--0.036100       0     3.02418  -3.13804   12.16402  L
H-HC-0.100000        0     1.49468  -5.73218   11.5493  L
H-HC-0.100000        0     0.78055  -4.12038   11.7757  L
H-HC-0.100000        0     1.54384  -4.91898   13.13282  L
H-HC-0.100000        0     3.93652  -5.08739   13.30122  L
H-HC-0.100000        0     5.01673  -4.55316   12.01556  L
H-HC-0.100000        0     3.98518  -5.99558   11.7823  L
N-N--0.516300        0     2.98343  -0.82913   9.0466   L
C-CT-0.039700        -1    3.10976   0.62498   9.29076  L
C-C-0.536600         0     1.84497   1.46687   9.0086   L
O-O--0.581900        0     1.89557   2.69658   9.07948  L
C-CT-0.056000        0     4.33863   1.15756   8.51793  L
C-CT-0.013600        0     4.29224   1.01887   6.98332  L
C-C-0.805400         0     4.91213  -0.28626   6.46787  L
O-O2--0.818800       0     4.26459  -1.36091   6.50679  L
O-O2--0.818800       0     6.10075  -0.28379   6.05738  L
H-H-0.293600         0     3.30672  -1.19265   8.15426  L
H-H1-0.110500        0     3.30962   0.77263   10.35286  L
H-HC--0.017300       0     5.23433   0.65579   8.88836  L
H-HC--0.017300       0     4.45556   2.21501   8.75755  L
H-HC--0.042500       0     4.86107   1.8449    6.55528  L
H-HC--0.042500       0     3.26632   1.11124   6.63698  L
N-N--0.415700        0     0.71476   0.81394   8.72865  L
C-CT--0.002400       -1   -0.60241   1.42979   8.5295   L
C-C-0.597300         0    -1.73393   0.77534   9.33795  L
O-O--0.567900        0    -2.91535   1.06652   9.14255  L
C-CT--0.034300       0    -0.97876   1.28231   7.04198  L
C-CA-0.011800        0    -0.03371   1.82566   5.98478  L
C-CA--0.125600       0    -0.19988   3.13843   5.51348  L
C-CA--0.125600       0     0.91584   0.98619   5.36952  L
C-CA--0.170400       0     0.56019   3.59944   4.42678  L
C-CA--0.170400       0     1.71558   1.46541   4.31494  L
C-CA--0.107200       0     1.54116   2.77802   3.84522  L
H-H-0.271900         0     0.7878   -0.18623   8.59197  L
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H-H1-0.097800        0    -0.56839   2.48883   8.78687  L
H-HC-0.029500        0    -1.94373   1.76319   6.88461  L
H-HC-0.029500        0    -1.12544   0.22011   6.84821  L
H-HA-0.133000        0    -0.93372   3.78832   5.96806  L
H-HA-0.133000        0     1.02507  -0.0339    5.70428  L
H-HA-0.143000        0     0.37945   4.59537   4.05576  L
H-HA-0.143000        0     2.44877   0.81912   3.85486  L
H-HA-0.129700        0     2.15404   3.15082   3.03653  L
N-N--0.415700        0    -1.36703  -0.12616   10.23617  L
C-CT--0.003100       -1   -2.22963  -0.99503   11.01854  L
C-C-0.597300         0    -3.4691   -0.29343   11.63141  L
O-O--0.567900        0    -4.61049  -0.64622   11.35097  L
C-CT--0.003600       0    -1.30562  -1.57729   12.10919  L
C-CT--0.064500       0    -1.95847  -2.31262   13.29257  L
C-C-0.695100         0    -1.02649  -2.33591   14.50313  L
O-O--0.608600        0    -0.55798  -3.37585   14.93815  L
N-N--0.940700        0    -0.71998  -1.20522   15.1081  L
H-H-0.271900         0    -0.37045  -0.18843   10.40387  L
H-H1-0.085000        0    -2.60616  -1.80003   10.40114  L
H-HC-0.017100        0    -0.72383  -0.74884   12.51667  L
H-HC-0.017100        0    -0.59841  -2.25653   11.63498  L
H-HC-0.035200        0    -2.19938  -3.3329    12.99305  L
H-HC-0.035200        0    -2.87923  -1.82633   13.60675  L
H-H-0.425100         0    -0.08446  -1.31079   15.87209  L
H-H-0.425100         0    -0.99818  -0.27708   14.77763  L
N-N--0.516300        0    -3.2502    0.6402    12.55199  L
C-CT-0.038100        -1   -4.23554   1.49566   13.25208  L
C-C-0.536600         0    -4.78745   2.59359   12.34066  L
O-O--0.581900        0    -5.95933   2.95268   12.45068  L
C-CT--0.030300       0    -3.54215   2.10277   14.48737  L
C-C-0.799400         0    -2.08708   2.45935   14.17269  L
O-O2--0.801400       0    -1.85659   3.49282   13.50846  L
O-O2--0.801400       0    -1.22487   1.56792   14.37442  L
H-H-0.293600         0    -2.27171   0.81142   12.75963  L
H-H1-0.088000        0    -5.08138   0.89243   13.58287  L
H-HC--0.012200       0    -3.5569    1.36467   15.29147  L
H-HC--0.012200       0    -4.08479   2.98598   14.82857  L
N-N--0.415700        0    -3.95789   3.09352   11.41773  L
C-CT-0.014300        -1   -4.32881   4.12061   10.44789  L
C-C-0.597300         0    -5.6126    3.78139   9.69138  L
O-O--0.567900        0    -6.42938   4.65802   9.41062  L
C-CT--0.204100       0    -3.20024   4.38293   9.42603  L
C-C-0.713000         0    -1.93006   5.07088   9.89904  L
O-O--0.593100        0    -1.25532   5.70969   9.10614  L
N-N--0.919100        0    -1.49771   4.95983   11.13465  L
H-H-0.271900         0    -3.019     2.72379   11.41367  L
H-H1-0.104800        0    -4.52711   5.04934   10.98591  L
H-HC-0.079700        0    -3.61587   5.02975   8.65071  L
H-HC-0.079700        0    -2.91914   3.4648    8.92669  L
H-H-0.419600         0    -0.66163   5.48571   11.2996  L
H-H-0.419600         0    -1.94851   4.45849   11.90248  L
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N-N--0.347900        0    -5.78326   2.495     9.37271  L
C-CT--0.263700       -1   -6.91289   1.97587   8.60939  L
C-C-0.734100         0    -8.31513   2.27102   9.16315  L
O-O--0.589400        0    -9.30113   2.05174   8.46195  L
C-CT--0.000700       0    -6.71413   0.47568   8.32678  L
C-CT-0.039000        0    -7.30217  -0.41454   9.42649  L
C-CT-0.048600        0    -6.88384  -1.87332   9.2666   L
N-N2--0.529500       0    -7.55957  -2.67606   10.29268  L
C-CA-0.807600        0    -7.05337  -3.04892   11.44291  L
N-N2--0.862700       0    -5.78188  -3.13936   11.67258  L
N-N2--0.862700       0    -7.84169  -3.28572   12.44192  L
H-H-0.274700         0    -5.0275    1.86891   9.62949  L
H-H1-0.156000        0    -6.88221   2.48476   7.64363  L
H-HC-0.032700        0    -5.64842   0.26566   8.21832  L
H-HC-0.032700        0    -7.20899   0.22801   7.38618  L
H-HC-0.028500        0    -8.39139  -0.3648    9.39073  L
H-HC-0.028500        0    -6.97006  -0.05437   10.40063  L
H-H1-0.068700        0    -5.8023   -1.93141   9.36521  L
H-H1-0.068700        0    -7.16064  -2.23796   8.2806   L
H-H-0.345600         0    -8.56771  -2.74399   10.23573  L
H-H-0.447800         0    -5.41317  -2.20026   11.77319  L
H-H-0.447800         0    -5.3009   -3.49199   10.83527  L
H-H-0.447800         0    -7.4137   -3.51776   13.31288  L
H-H-0.447800         0    -8.81629  -3.00461   12.3399  L
N-N--0.415700        0    -8.43459   2.73749   10.40306  L
C-CT--0.149000       -1   -9.71297   3.0927    10.98943  L
H-H-0.271900         0    -7.57832   2.89775   10.92105  L
H-H1-0.097600        0    -10.29551   3.69458   10.29089  L
H-H1-0.097600        0    -9.54986   3.66167   11.90541  L
H-H1-0.097600        0    -10.2666   2.18196   11.22682  L
C-CT--0.366200       -1   -9.93038   6.29408   8.78261  L
C-C-0.597200         0    -10.64698   5.54508   7.68393  L
O-O--0.567900        0    -11.83008   5.78612   7.48393  L
H-HC-0.112300        0    -9.12335   5.68493   9.19021  L
H-HC-0.112300        0    -10.64017   6.53901   9.56964  L
H-HC-0.112300        0    -9.51558   7.20998   8.36567  L
N-N--0.415700        0    -9.95514   4.62851   7.0033   L
C-CT--0.001400       -1   -10.4793   3.77948   5.91294  L
C-C-0.597300         0    -11.81074   3.07877   6.22102  L
O-O--0.567900        0    -12.68728   2.93593   5.36568  L
C-CT--0.015200       0    -9.34162   2.88154   5.37137  L
C-CA--0.001100       0    -9.72892   1.64125   4.586    L
C-CA--0.190600       0    -10.34623   0.5614    5.24613  L
C-CA--0.190600       0    -9.40526   1.53177   3.21844  L
C-CA--0.234100       0    -10.69367  -0.59662   4.53105  L
C-CA--0.234100       0    -9.71011   0.35388   2.50763  L
C-C-0.322600         0    -10.36525  -0.70605   3.16508  L
O-OH--0.557900       0    -10.69521  -1.83611   2.49597  L
H-H-0.271900         0    -8.98476   4.51241   7.25449  L
H-H1-0.087600        0    -10.72791   4.45569   5.0933   L
H-HC-0.029500        0    -8.70736   2.55142   6.18655  L
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H-HC-0.029500        0    -8.70357   3.50465   4.74332  L
H-HA-0.169900        0    -10.56274   0.62968   6.30266  L
H-HA-0.169900        0    -8.90707   2.34767   2.71249  L
H-HA-0.165600        0    -11.19828  -1.4099    5.0237   L
H-HA-0.165600        0    -9.46103   0.25344   1.4597   L
H-HO-0.399200        0    -11.60443  -2.06387   2.75799  L
N-N--0.516300        0    -11.97683   2.66406   7.46947  L
C-CT-0.038100        -1   -13.20221   2.09631   8.00866  L
C-C-0.536600         0    -14.40779   3.05325   8.1647   L
O-O--0.581900        0    -15.54183   2.55652   8.21447  L
C-CT--0.030300       0    -12.87294   1.53715   9.41689  L
C-C-0.799400         0    -12.16977   0.17468   9.41922  L
O-O2--0.801400       0    -12.67658  -0.74406   8.73609  L
O-O2--0.801400       0    -11.182   -0.02989   10.15356  L
H-H-0.293600         0    -11.14663   2.71692   8.05206  L
H-H1-0.088000        0    -13.52067   1.27732   7.36355  L
H-HC--0.012200       0    -13.8018   1.41149   9.97524  L
H-HC--0.012200       0    -12.27635   2.26691   9.96499  L
N-N--0.415700        0    -14.17136   4.36405   8.34589  L
C-CT--0.149000       -1   -15.12221   5.40631   8.76152  L
H-H-0.271900         0    -13.21829   4.6659    8.15866  L
H-H1-0.097600        0    -16.0274   5.33693   8.15619  L
H-H1-0.097600        0    -14.66937   6.38877   8.61694  L
H-H1-0.097600        0    -15.37992   5.27388   9.81263  L
C-CT--0.366200       -1   -19.77902  -1.20428  -1.31362  L
C-C-0.597200         0    -18.78733  -0.84147  -0.19673  L
O-O--0.567900        0    -18.41572   0.322    -0.11262  L
H-HC-0.112300        0    -20.62574  -1.74014  -0.89196  L
H-HC-0.112300        0    -19.26705  -1.81877  -2.0528   L
H-HC-0.112300        0    -20.12208  -0.28688  -1.79019  L
N-N--0.415700        0    -18.34804  -1.78329   0.66773  L
C-CT--0.058100       -1   -17.22251  -1.55438   1.62381  L
C-C-0.597300         0    -16.37264  -2.78248   1.96377  L
O-O--0.567900        0    -16.79592  -3.60338   2.78259  L
C-CT--0.007400       0    -17.66302  -0.77647   2.87491  L
C-CC-0.186800        0    -16.48184  -0.03117   3.45193  L
N-NB--0.543200       0    -15.43628  -0.62907   4.14666  L
C-CW--0.220700       0    -16.16022   1.27661   3.22417  L
C-CR-0.163500        0    -14.48188   0.30886   4.28179  L
N-NA--0.279500       0    -14.91013   1.47747   3.78116  L
H-H-0.271900         0    -18.69115  -2.72375   0.55518  L
H-H1-0.136000        0    -16.56894  -0.85017   1.11425  L
H-HC-0.036700        0    -18.07844  -1.45511   3.62019  L
H-HC-0.036700        0    -18.42833  -0.04764   2.60642  L
H-H4-0.186200        0    -16.7377   1.98272   2.64116  L
H-H-0.333900         0    -14.34412   2.32446   3.79338  L
H-H5-0.143500        0    -13.51043   0.15668   4.73867  L
N-N--0.254800        0    -15.16916  -2.91057   1.37446  L
C-CT--0.026600       -1   -14.212   -3.9216    1.79001  L
C-C-0.589600         0    -13.52668  -3.58404   3.10448  L
O-O--0.574800        0    -13.14535  -2.43839   3.34469  L
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C-CT--0.007000       0    -13.16064  -3.96403   0.68937  L
C-CT-0.018900        0    -13.19439  -2.5751    0.05402  L
C-CT-0.019200        0    -14.6403  -2.13263   0.25279  L
H-H1-0.064100        0    -14.69873  -4.89448   1.86946  L
H-HC-0.025300        0    -13.47887  -4.7075   -0.02495  L
H-HC-0.025300        0    -12.16797  -4.21359   1.06752  L
H-HC-0.021300        0    -12.92196  -2.60014  -1.00149  L
H-HC-0.021300        0    -12.53374  -1.89975   0.59567  L
H-H1-0.039100        0    -14.65191  -1.06172   0.45727  L
H-H1-0.039100        0    -15.21639  -2.35352  -0.64728  L
N-N--0.347900        0    -13.24752  -4.59958   3.92357  L
C-CT--0.263700       -1   -12.4845  -4.41253   5.16445  L
C-C-0.734100         0    -10.9741  -4.7534    4.99205  L
O-O--0.589400        0    -10.64846  -5.61214   4.1781   L
C-CT--0.000700       0    -13.20711  -5.05697   6.36005  L
C-CT-0.039000        0    -14.52543  -4.3085    6.68327  L
C-CT-0.048600        0    -14.31189  -2.92165   7.32945  L
N-N2--0.529500       0    -15.22941  -1.88199   6.80679  L
C-CA-0.807600        0    -15.64333  -0.78287   7.42248  L
N-N2--0.862700       0    -15.35721  -0.50974   8.65501  L
N-N2--0.862700       0    -16.32076   0.13227   6.79861  L
H-H-0.274700         0    -13.50354  -5.52956   3.61704  L
H-H1-0.156000        0    -12.46091  -3.34615   5.37918  L
H-HC-0.032700        0    -12.55903  -5.03564   7.23815  L
H-HC-0.032700        0    -13.43051  -6.098     6.12313  L
H-HC-0.028500        0    -15.10999  -4.9164    7.37443  L
H-HC-0.028500        0    -15.11382  -4.20294   5.77059  L
H-H1-0.068700        0    -13.29188  -2.58943   7.142    L
H-H1-0.068700        0    -14.42546  -3.02153   8.4104   L
H-H-0.345600         0    -15.4201  -1.89388   5.80979  L
H-H-0.447800         0    -15.58703   0.41444   8.97586  L
H-H-0.447800         0    -14.46523  -0.92342   8.92851  L
H-H-0.447800         0    -16.39805   1.04792   7.22529  L
H-H-0.447800         0    -16.35766   0.04189   5.78997  L
N-N--0.415700        0    -10.04942  -4.03475   5.6609   L
C-CT--0.003100       -1   -8.56298  -4.13617   5.5428   L
C-C-0.597300         0    -7.96183  -4.96702   6.68338  L
O-O--0.567900        0    -8.41697  -4.88637   7.82613  L
C-CT--0.003600       0    -7.93698  -2.73578   5.49881  L
C-CT--0.064500       0    -6.40312  -2.80802   5.4013   L
C-C-0.695100         0    -5.8194   -1.48211   4.96628  L
O-O--0.608600        0    -6.07407  -1.04856   3.85584  L
N-N--0.940700        0    -5.01555  -0.82608   5.76856  L
H-H-0.271900         0    -10.39546  -3.34548   6.31847  L
H-H1-0.085000        0    -8.33746  -4.64663   4.61243  L
H-HC-0.017100        0    -8.21702  -2.17265   6.38747  L
H-HC-0.017100        0    -8.3315   -2.2028    4.63575  L
H-HC-0.035200        0    -6.11499  -3.55037   4.65782  L
H-HC-0.035200        0    -5.98692  -3.09955   6.36297  L
H-H-0.425100         0    -4.74395   0.11535   5.5104   L
H-H-0.425100         0    -4.6823   -1.28911   6.62468  L
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N-N--0.415700        0    -6.90502  -5.72068   6.37437  L
C-CT--0.001400       -1   -6.15637  -6.53876   7.32359  L
C-C-0.597300         0    -4.65315  -6.47927   7.03103  L
O-O--0.567900        0    -4.21343  -6.65613   5.88903  L
C-CT--0.015200       0    -6.63656  -8.00215   7.26996  L
C-CA--0.001100       0    -8.13371  -8.19295   7.10849  L
C-CA--0.190600       0    -8.97757  -8.35551   8.22649  L
C-CA--0.190600       0    -8.68269  -8.1573    5.81375  L
C-CA--0.234100       0    -10.37015  -8.49701   8.04449  L
C-CA--0.234100       0    -10.06839  -8.27344   5.63757  L
C-C-0.322600         0    -10.91612  -8.45963   6.74349  L
O-OH--0.557900       0    -12.24945  -8.6078    6.53349  L
H-H-0.271900         0    -6.62111  -5.7633    5.40002  L
H-H1-0.087600        0    -6.32881  -6.1554    8.33046  L
H-HC-0.029500        0    -6.30326  -8.5117    8.17468  L
H-HC-0.029500        0    -6.15189  -8.49787   6.42708  L
H-HA-0.169900        0    -8.55823  -8.35589   9.22202  L
H-HA-0.169900        0    -8.04397  -7.99589   4.95475  L
H-HA-0.165600        0    -11.03315  -8.62177   8.88584  L
H-HA-0.165600        0    -10.4915  -8.18514   4.65498  L
H-HO-0.399200        0    -12.38941  -8.71383   5.58016  L
N-N--0.516300        0    -3.851    -6.24696   8.06765  L
C-CT-0.039700        -1   -2.4008   -6.16453   7.93769  L
C-C-0.536600         0    -1.70442  -7.53381   8.01978  L
O-O--0.581900        0    -1.9211   -8.31525   8.94614  L
C-CT-0.056000        0    -1.78711  -5.17002   8.93143  L
C-CT-0.013600        0    -2.05442  -3.71756   8.5078   L
C-C-0.805400         0    -3.53524  -3.31193   8.60269  L
O-O2--0.818800       0    -4.22803  -3.79386   9.53246  L
O-O2--0.818800       0    -3.98707  -2.51413   7.75201  L
H-H-0.293600         0    -4.26272  -5.93646   8.93985  L
H-H1-0.110500        0    -2.1963   -5.77045   6.94868  L
H-HC--0.017300       0    -0.70479  -5.31228   8.93644  L
H-HC--0.017300       0    -2.15517  -5.35757   9.94114  L
H-HC--0.042500       0    -1.69978  -3.58318   7.48386  L
H-HC--0.042500       0    -1.44959  -3.06845   9.14096  L
N-N--0.415700        0    -0.81775  -7.81553   7.05876  L
C-CT--0.002400       -1   -0.0565   -9.06774   6.95576  L
C-C-0.597300         0     1.4462   -8.83111   7.12976  L
O-O--0.567900        0     1.96204  -7.70928   7.15614  L
C-CT--0.034300       0    -0.40178  -9.75595   5.61572  L
C-CA-0.011800        0     0.15142  -9.06961   4.37431  L
C-CA--0.125600       0    -0.5803   -8.05848   3.72618  L
C-CA--0.125600       0     1.42406  -9.41587   3.88524  L
C-CA--0.170400       0    -0.01113  -7.3516    2.65007  L
C-CA--0.170400       0     1.99664  -8.70897   2.81227  L
C-CA--0.107200       0     1.2787   -7.67043   2.1973   L
H-H-0.271900         0    -0.68918  -7.1131    6.33496  L
H-H1-0.097800        0    -0.37682  -9.73239   7.75888  L
H-HC-0.029500        0    -1.48763  -9.82418   5.5265   L
H-HC-0.029500        0    -0.02455  -10.77854   5.64186  L
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H-HA-0.133000        0    -1.56206  -7.78326   4.08827  L
H-HA-0.133000        0     1.9678   -10.21994   4.3498   L
H-HA-0.143000        0    -0.54839  -6.53243   2.19312  L
H-HA-0.143000        0     2.98732  -8.95608   2.46393  L
H-HA-0.129700        0     1.71249  -7.10337   1.38665  L
N-N--0.415700        0     2.17971  -9.93263   7.27221  L
C-CT--0.024900       -1    3.62344  -9.8828    7.462    L
C-C-0.597300         0     4.37469  -9.39402   6.2067   L
O-O--0.567900        0     4.24938  -9.96102   5.12344  L
C-CT-0.211700        0     4.16935  -11.25667   7.89125  L
O-OH--0.654600       0     3.92652  -12.28524   6.93737  L
H-H-0.271900         0     1.69878  -10.81406   7.20917  L
H-H1-0.084300        0     3.82969  -9.18263   8.2725   L
H-H1-0.035200        0     3.71562  -11.53829   8.84305  L
H-H1-0.035200        0     5.24624  -11.16961   8.04489  L
H-HO-0.427500        0     3.14844  -12.77773   7.22854  L
N-N--0.347900        0     5.22953  -8.37712   6.34834  L
C-CT--0.263700       -1    6.11661  -7.85532   5.28427  L
C-C-0.734100         0     7.20212  -8.85019   4.83824  L
O-O--0.589400        0     7.26731  -9.9855    5.31543  L
C-CT--0.000700       0     6.67051  -6.50204   5.78245  L
C-CT-0.039000        0     7.79493  -6.60118   6.82814  L
C-CT-0.048600        0     8.11087  -5.25046   7.487    L
N-N2--0.529500       0     8.414    -4.17954   6.51211  L
C-CA-0.807600        0     7.64577  -3.15205   6.189    L
N-N2--0.862700       0     6.43334  -3.04955   6.63893  L
N-N2--0.862700       0     8.06516  -2.18807   5.42753  L
H-H-0.274700         0     5.22249  -7.92406   7.24871  L
H-H1-0.156000        0     5.49422  -7.65862   4.4083   L
H-HC-0.032700        0     5.84327  -5.92349   6.19832  L
H-HC-0.032700        0     7.05225  -5.9372    4.94098  L
H-HC-0.028500        0     8.6995   -6.97446   6.35097  L
H-HC-0.028500        0     7.50559  -7.30287   7.611    L
H-H1-0.068700        0     8.97717  -5.38424   8.13685  L
H-H1-0.068700        0     7.27329  -4.96373   8.12436  L
H-H-0.345600         0     9.34469  -4.17744   6.10216  L
H-H-0.447800         0     5.88516  -2.21272   6.39593  L
H-H-0.447800         0     6.02735  -3.72106   7.24693  L
H-H-0.447800         0     7.39942  -1.41854   5.31512  L
H-H-0.447800         0     8.96382  -2.17866   4.97303  L
N-N--0.415700        0     8.07113  -8.41039   3.9349   L
C-CT--0.051800       -1    9.41093  -8.94846   3.68376  L
C-C-0.597300         0     10.32974  -7.73983   3.85761  L
O-O--0.567900        0     10.36936  -6.84104   3.02209  L
C-CT--0.110200       0     9.43716  -9.59041   2.28121  L
C-CT-0.353100        0     10.7694  -10.24606   1.86257  L
C-CT--0.412100       0     10.4953  -11.32614   0.81307  L
C-CT--0.412100       0     11.75698  -9.26647   1.23064  L
H-H-0.271900         0     7.88678  -7.49586   3.52767  L
H-H1-0.092200        0     9.6669   -9.70644   4.4265   L
H-HC-0.045700        0     9.14003  -8.8591    1.52819  L
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H-HC-0.045700        0     8.67963  -10.36842   2.28867  L
H-HC--0.036100       0     11.23012  -10.71692   2.73119  L
H-HC-0.100000        0     11.43215  -11.79951   0.51748  L
H-HC-0.100000        0     10.03118  -10.88008  -0.06874  L
H-HC-0.100000        0     9.83876  -12.09205   1.22302  L
H-HC-0.100000        0     12.65194  -9.8009    0.91429  L
H-HC-0.100000        0     12.04981  -8.49981   1.93987  L
H-HC-0.100000        0     11.30315  -8.78916   0.36333  L
N-N--0.415700        0     11.01394  -7.67441   4.99334  L
C-CT-0.014300        -1    12.2925  -6.99003   5.02217  L
C-C-0.597300         0     13.33205  -8.05222   4.57519  L
O-O--0.567900        0     13.3322  -9.13524   5.16121  L
C-CT--0.204100       0     12.6381  -6.49957   6.43893  L
C-C-0.713000         0     11.83055  -5.30959   6.9144   L
O-O--0.593100        0     11.15618  -4.61281   6.17332  L
N-N--0.919100        0     11.87376  -5.02837   8.19498  L
H-H-0.271900         0     10.9402  -8.46548   5.61498  L
H-H1-0.104800        0     12.31423  -6.15126   4.32437  L
H-HC-0.079700        0     13.68756  -6.20129   6.44901  L
H-HC-0.079700        0     12.51897  -7.32204   7.14458  L
H-H-0.419600         0     11.38686  -4.2011    8.4833   L
H-H-0.419600         0     12.46936  -5.56098   8.80753  L
N-N--0.415700        0     14.15753  -7.81185   3.54557  L
C-CT--0.051800       -1    15.26379  -8.72038   3.18548  L
C-C-0.597300         0     16.47631  -8.49058   4.12633  L
O-O--0.567900        0     16.74084  -7.35071   4.50484  L
C-CT--0.110200       0     15.63334  -8.58012   1.67455  L
C-CT-0.353100        0     16.65197  -9.61136   1.10394  L
C-CT--0.412100       0     16.16001  -11.05056   1.29727  L
C-CT--0.412100       -1    16.93258  -9.45704  -0.41113  L
H-H-0.271900         0     14.12037  -6.92025   3.07374  L
H-H1-0.092200        0     14.91545  -9.73909   3.35143  L
H-HC-0.045700        0     16.03675  -7.582     1.50878  L
H-HC-0.045700        0     14.71845  -8.65691   1.08885  L
H-HC--0.036100       0     17.5961  -9.49777   1.63199  L
H-HC-0.100000        0     15.18237  -11.17809   0.83295  L
H-HC-0.100000        0     16.09785  -11.29359   2.35544  L
H-HC-0.100000        0     16.86776  -11.74261   0.84004  L
H-HC-0.100000        0     16.03557  -9.6803   -0.98476  L
H-HC-0.100000        0     17.73327  -10.13478  -0.70719  L
H-HC-0.100000        0     17.25527  -8.43439  -0.61052  L
N-N--0.516300        0     17.20765  -9.54533   4.51918  L
C-CT-0.039700        -1    18.46155  -9.41158   5.2998   L
C-C-0.536600         0     19.54172  -8.60578   4.52089  L
O-O--0.581900        0     19.47274  -8.48396   3.29476  L
C-CT-0.056000        0     18.99828  -10.77904   5.76478  L
C-CT-0.013600        0     18.69684  -11.03597   7.25152  L
C-C-0.805400         0     19.2398  -9.93751   8.18789  L
O-O2--0.818800       0     18.69292  -9.81737   9.30409  L
O-O2--0.818800       0     20.14319  -9.181     7.75433  L
H-H-0.293600         0     16.95834  -10.46029   4.18767  L
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H-H1-0.110500        0     18.22568  -8.80364   6.17399  L
H-HC--0.017300       0     20.07888  -10.82089   5.62009  L
H-HC--0.017300       0     18.55812  -11.57663   5.16348  L
H-HC--0.042500       0     19.13314  -11.99736   7.53156  L
H-HC--0.042500       0     17.61317  -11.11359   7.37026  L
N-N--0.415700        0     20.50647  -7.98225   5.21573  L
C-CT--0.025200       -1    21.5108  -7.04729   4.64629  L
C-C-0.597300         0     20.89207  -5.78302   3.98459  L
O-O--0.567900        0     21.63733  -5.0157    3.37941  L
H-H-0.271900         0     20.52832  -8.19643   6.21723  L
H-H1-0.069800        0     22.0951  -7.57084   3.88976  L
H-H1-0.069800        0     22.18519  -6.72245   5.43773  L
N-N--0.415700        0     19.56649  -5.53367   4.0672   L
C-CT--0.038900       0     18.8294  -4.63369   3.13932  L
C-C-0.597300         0     17.86488  -3.63125   3.81632  L
O-O--0.567900        0     17.04854  -3.97699   4.66799  L
C-CT-0.365400        0     18.03163  -5.4603    2.10809  L
O-OH--0.676100       0     18.80439  -6.48535   1.52455  L
C-CT--0.243800       0     17.55707  -4.61955   0.92107  L
H-H-0.271900         0     19.01122  -6.19166   4.59907  L
H-H1-0.100700        0     19.56336  -4.05741   2.5774   L
H-H1-0.004300        0     17.16174  -5.89941   2.58997  L
H-HC-0.064200        0     16.89511  -3.82315   1.25145  L
H-HC-0.064200        0     17.01094  -5.25813   0.22654  L
H-HC-0.064200        0     18.41612  -4.19028   0.40486  L
H-HO-0.410200        0     19.03925  -7.13917   2.21016  L
N-N--0.415700        0     17.90095  -2.36121   3.38672  L
C-CT--0.087500       -1    16.98934  -1.25787   3.78802  L
C-C-0.597300         0     15.62657  -1.40245   3.07372  L
O-O--0.567900        0     15.58159  -1.43429   1.84741  L
C-CT-0.298500        0     17.58063   0.11284   3.37743  L
C-CT--0.319200       -1    16.71002   1.31502   3.84195  L
C-CT--0.319200       -1    19.02704   0.21637   3.8953   L
H-H-0.271900         0     18.57684  -2.15909   2.66531  L
H-H1-0.096900        0     16.84587  -1.28199   4.86756  L
H-HC--0.029700       0     17.63865   0.15853   2.28955  L
H-HC-0.079100        0     16.58094   1.29253   4.9231   L
H-HC-0.079100        0     15.74053   1.30314   3.3445   L
H-HC-0.079100        0     17.2253   2.23391   3.56668  L
H-HC-0.079100        0     19.05408   0.0481    4.97204  L
H-HC-0.079100        0     19.41446   1.21382   3.6851   L
H-HC-0.079100        0     19.67822  -0.50057   3.39599  L
N-N--0.415700        0     14.50432  -1.50314   3.80505  L
C-CT--0.023700       -1    13.20214  -1.94511   3.23894  L
C-C-0.597300         0     11.93276  -1.30273   3.87957  L
O-O--0.567900        0     10.82545  -1.85087   3.81303  L
C-CT-0.034200        0     13.09692  -3.47571   3.4758   L
C-CT-0.001800        0     14.18457  -4.38827   2.88571  L
S-S--0.273700        0     13.7107  -5.28904   1.38584  L
C-CT--0.053600       0     13.79105  -3.94136   0.18203  L
H-H-0.271900         0     14.64105  -1.55887   4.80159  L
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 H-H1-0.088000        0     13.16539  -1.74735   2.16694  L
 H-HC-0.024100        0     12.13808  -3.83901   3.10337  L
 H-HC-0.024100        0     13.09972  -3.6355    4.55458  L
 H-H1-0.044000        0     14.43702  -5.12715   3.64548  L
 H-H1-0.044000        0     15.09662  -3.83585   2.68789  L
 H-H1-0.068400        0     14.78321  -3.48979   0.19364  L
 H-H1-0.068400        0     13.04796  -3.18282   0.42353  L
 H-H1-0.068400        0     13.58948  -4.34153  -0.8089   L
 N-N--0.415700        0     12.06386  -0.13071   4.50619  L
 C-CT--0.024900       -1    10.94652   0.78759   4.81705  L
 C-C-0.597300         0     11.03046   1.89218   3.76933  L
 O-O--0.567900        0     12.12728   2.40631   3.54521  L
 C-CT-0.211700        0     11.07543   1.30358   6.24651  L
 O-OH--0.654600       0     10.13156   2.30522   6.56163  L
 H-H-0.271900         0     12.97638   0.2951    4.425    L
 H-H1-0.084300        0     9.98877   0.27675   4.71516  L
 H-H1-0.035200        0     12.07458   1.70983   6.37492  L
 H-H1-0.035200        0     10.94708   0.46636   6.93364  L
 H-HO-0.427500        0     9.24731   2.04399   6.21006  L
 N-N--0.347900        0     9.93877   2.19257   3.0519   L
 C-CT--0.240000       -1    9.99026   3.0891    1.88191  L
 C-C-0.734100         0     10.5708   4.46263   2.2846   L
 O-O--0.589400        0     11.58745   4.84367   1.71174  L
 C-CT--0.009400       0     8.61129   3.16016   1.17342  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.63505   3.70744  -0.27542  H
 C-CT--0.047900       0     7.37969   3.27057  -1.05276  H
 C-CT--0.014300       0     7.24675   3.91453  -2.42904  H
 N-N3--0.385400       0     6.01532   3.4019   -3.1581   H
 H-H-0.274700         0     9.0577    1.75996   3.30842  L
 H-H1-0.142600        0     10.69969   2.66388   1.17049  L
 H-HC-0.036200        0     7.92946   3.77423   1.76165  L
 H-HC-0.036200        0     8.20228   2.14831   1.14133  L
 H-HC-0.010300        0     9.53129   3.33131  -0.77795  H
 H-HC-0.010300        0     8.70155   4.79885  -0.22637  H
 H-HC-0.062100        0     6.47177   3.52775  -0.50483  H
 H-HC-0.062100        0     7.37591   2.18303  -1.17417  H
 H-HP-0.113500        0     8.08714   3.73365  -3.10409  H
 H-HP-0.113500        0     7.10313   4.99464  -2.34692  H
 H-H-0.340000         0     6.20907   2.64192  -3.82273  H
 H-H-0.340000         0     5.6237    4.12935  -3.79193  H
 H-H-0.340000         0     5.23136   3.09934  -2.52909  H
 N-N--0.347900        0     10.08101   5.09013   3.37813  L
 C-CT--0.263700       -1    10.63694   6.2906    4.0968   L
 C-C-0.734100         0     11.94605   6.07024   4.83888  L
 O-O--0.589400        0     12.22372   6.71605   5.84622  L
 C-CT--0.000700       0     9.51915   6.93253   4.95211  L
 C-CT-0.039000        0     8.32238   7.36395   4.07543  L
 C-CT-0.048600        0     7.47662   8.48814   4.68782  L
 N-N2--0.529500       0     6.45352   8.02737   5.65308  L
 C-CA-0.807600        0     5.19696   8.44568   5.69708  L
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N-N2--0.862700       0     4.63374   9.06935   4.70803  L
N-N2--0.862700       0     4.49525   8.24747   6.76751  L
H-H-0.274700         0     9.24176   4.66375   3.74509  L
H-H1-0.156000        0     10.908    7.02473   3.33217  L
H-HC-0.032700        0     9.92699   7.81991   5.43902  L
H-HC-0.032700        0     9.18232   6.23736   5.72271  L
H-HC-0.028500        0     7.687     6.5067    3.84571  L
H-HC-0.028500        0     8.71167   7.74962   3.13179  L
H-H1-0.068700        0     6.9972    9.01199   3.86243  L
H-H1-0.068700        0     8.13145   9.21401   5.17192  L
H-H-0.345600         0     6.73812   7.49672   6.45639  L
H-H-0.447800         0     3.68104   9.43354   4.74481  L
H-H-0.447800         0     5.073     8.96319   3.80026  L
H-H-0.447800         0     3.54091   8.61097   6.79688  L
H-H-0.447800         0     4.82641   7.67289   7.52927  L
N-N--0.347900        0     12.74636   5.14975   4.30611  L
C-CT--0.240000       -1    14.13066   4.841     4.65508  L
C-C-0.734100         0     14.99762   4.48286   3.41846  L
O-O--0.589400        0     16.2155   4.49918   3.54102  L
C-CT--0.009400       0     14.22726   3.77537   5.77573  L
C-CT-0.018700        0     13.37255   4.17722   6.99165  L
C-CT--0.047900       0     13.46871   3.31836   8.25441  L
C-CT--0.014300       0     12.27166   3.75356   9.11753  L
N-N3--0.385400       0     12.20165   3.04665   10.41763  L
H-H-0.274700         0     12.35573   4.71948   3.48108  L
H-H1-0.142600        0     14.57953   5.75751   5.04438  L
H-HC-0.036200        0     15.26955   3.68855   6.08689  L
H-HC-0.036200        0     13.89981   2.80775   5.39793  L
H-HC-0.010300        0     12.32898   4.16308   6.6771   L
H-HC-0.010300        0     13.64063   5.1948    7.27823  L
H-HC-0.062100        0     14.41428   3.51834   8.76165  L
H-HC-0.062100        0     13.39798   2.26036   8.00454  L
H-HP-0.113500        0     11.35375   3.57171   8.54472  L
H-HP-0.113500        0     12.34023   4.83477   9.2797   L
H-H-0.340000         0     12.1013   2.05176   10.27104  L
H-H-0.340000         0     11.39675   3.37382   10.93919  L
H-H-0.340000         0     13.03444   3.22627   10.96274  L
N-N--0.415700        0     14.40604   4.17169   2.25153  L
C-CT--0.051800       -1    15.05245   3.7147    0.99411  L
C-C-0.597300         0     15.26004   4.8031   -0.02612  L
O-O--0.567900        0     16.23205   4.77493  -0.77904  L
C-CT--0.110200       0     14.20014   2.54739   0.45193  L
C-CT-0.353100        0     14.72815   1.86074  -0.8228   L
C-CT--0.412100       0     16.1212   1.25849  -0.63374  L
C-CT--0.412100       0     13.77452   0.72861  -1.21411  L
H-H-0.271900         0     13.39663   4.21347   2.23734  L
H-H1-0.092200        0     16.04213   3.32956   1.2443   L
H-HC-0.045700        0     13.19743   2.92416   0.24345  L
H-HC-0.045700        0     14.11418   1.79304   1.23595  L
H-HC--0.036100       0     14.75694   2.58005  -1.64058  L
H-HC-0.100000        0     16.12193   0.566     0.20692  L
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H-HC-0.100000        0     16.84844   2.05009  -0.4558   L
H-HC-0.100000        0     16.41717   0.72627  -1.5373   L
H-HC-0.100000        0     14.11434   0.27211  -2.14347  L
H-HC-0.100000        0     12.77198   1.12721  -1.36649  L
H-HC-0.100000        0     13.75009  -0.02957  -0.43028  L
N-N--0.415700        0     14.35633   5.769    -0.03538  L
C-CT-0.014300        -1    14.56396   6.98519  -0.77491  L
C-C-0.597300         0     15.64141   7.91015  -0.13537  L
O-O--0.567900        0     15.34713   9.00141   0.34493  L
C-CT--0.204100       0     13.20075   7.66774  -1.06034  L
C-C-0.713000         0     12.2067    7.75876   0.0949   L
O-O--0.593100        0     12.52073   7.62492   1.26899  L
N-N--0.919100        0     10.94299   7.94216  -0.21815  L
H-H-0.271900         0     13.59996   5.75315   0.63905  L
H-H1-0.104800        0     14.96917   6.72004  -1.75303  L
H-HC-0.079700        0     12.71197   7.10924  -1.85811  L
H-HC-0.079700        0     13.37741   8.67732  -1.42971  L
H-H-0.419600         0     10.29414   7.97892   0.54287  L
H-H-0.419600         0     10.61715   8.02965  -1.17951  L
N-N--0.415700        0     16.91464   7.47971  -0.1853   L
C-CT--0.149000       -1    18.10715   8.18451   0.305    L
H-H-0.271900         0     17.02949   6.54848  -0.57202  L
H-H1-0.097600        0     18.03777   8.30744   1.3873   L
H-H1-0.097600        0     18.16445   9.17212  -0.15636  L
H-H1-0.097600        0     19.00553   7.61624   0.06138  L
C-CT--0.055800       0     1.0689    14.81614   4.42015  L
C-CT-0.000000        0     1.3999    13.87743   3.2615   L
O-OS--0.354800       0     2.80501   13.83763   3.04992  L
C-CT--0.202200       0     0.97405   12.44344   3.58057  L
O-OS--0.524600       0     0.47569   11.88044   2.36645  L
C-CT--0.067000       0     2.2849    11.8092   4.03189   L
O-OH--0.613900       0     2.24662   10.40684   3.92477  L
C-CT--0.006600       0     3.16324   12.46877   2.98527  L
N-N*--0.048400       0     4.61484   12.24247   3.1843   L
C-C-0.753800         0     5.30476   11.49256   2.22762  L
O-O--0.625200        0     4.72089   10.99901   1.26363  L
N-NC--0.758400       0     6.64255   11.29986   2.34977  L
C-CA-0.818500        0     7.25821   11.82334   3.38094  L
N-N2--0.953000       0     8.54294   11.61438   3.40507  L
C-CM--0.521500       0     6.61246   12.55884   4.4096   L
C-CM--0.005300       0     5.27454   12.74879   4.27608  L
H-H1-0.067900        0    -0.01391   14.86739   4.53793  L
H-H1-0.067900        0     1.51046   14.42892   5.3384   L
H-H1-0.117400        0     0.87324   14.21605   2.36539  L
H-H1-0.061500        0     0.20658   12.43825   4.35335  L
H-H1-0.097200        0     2.54802   12.13521   5.04041  L
H-HO-0.418600        0     1.51758   10.22037   3.30656  L
H-H2-0.202900        0     2.84561   12.06634   2.02005  L
H-H-0.423400         0     8.8708    11.16275   2.57054  L
H-H-0.423400         0     9.12074   12.06899   4.0812   L
H-HA-0.192800        0     7.13358   12.97271   5.25547  L
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 H-H4-0.195800        0     4.70843   13.31231   5.00914  L
 P-P-1.166200         0    -0.55536   10.64292   2.30909  L
 O-O2--0.776000       0    -1.55166   10.87024   1.24414  L
 O-O2--0.776000       0    -0.98905   10.30945   3.68289  L
 O-OS--0.498900       0     0.40001   9.43539   1.85534  L
 C-CT-0.055800        0     1.15593   9.48129   0.65581  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     1.99124   8.19404   0.49125  H
 O-OS--0.354800       0     2.67066   7.9864    1.71956  H
 C-CT-0.202200        0     1.22485   6.908     0.14342  H
 O-OH--0.654100       0     1.45974   6.46904  -1.17638  H
 C-CT-0.067000        0     1.77605   5.82043   1.14627  H
 O-OH--0.613900       0     2.4471    4.71762   0.59868  H
 C-CT-0.039400        0     2.76951   6.61296   2.0558   H
 N-N*--0.025100       0     2.46416   6.5186    3.46659  H
 C-CK-0.200600        0     1.36813   7.10673   4.07422  H
 N-NB--0.607300       0     1.25573   6.8228    5.3427   H
 C-CB-0.051500        0     2.32348   5.99222   5.5955   H
 C-CA-0.700900        0     2.69384   5.27593   6.74617  H
 N-N2--0.901900       0     2.00194   5.34354   7.92527  H
 N-NC--0.761500       0     3.84239   4.58213   6.72758  H
 C-CQ-0.587500        0     4.49392   4.48396   5.56264  H
 N-NC--0.699700       0     4.22211   5.05498   4.39174  H
 C-CB-0.305300        0     3.10887   5.79987   4.45419  H
 H-H1-0.067900        0     1.82896   10.33803   0.69968  L
 H-H1-0.067900        0     0.49002   9.60172  -0.20102  L
 H-H1-0.117400        0     2.71788   8.35342  -0.31915  H
 H-H1-0.061500        0     0.14975   7.04804   0.31414  H
 H-HO-0.437600        0     1.05338   7.0653   -1.83964  H
 H-H1-0.097200        0     0.93168   5.50743   1.77318  H
 H-HO-0.418600        0     4.06606   4.51307   0.98844  H
 H-H2-0.200700        0     3.7956    6.27568   1.90753  H
 H-H5-0.155300        0     0.69804   7.74675   3.51066  H
 H-H-0.411500         0     1.99882   4.45745   8.44272  H
 H-H-0.411500         0     1.04558   5.68521   7.82526  H
 H-H5-0.047300        0     5.3881    3.86719   5.57908  H
 N-N3-0.149300        0    -0.43986   4.41252  -0.25861  H
 C-CT-0.053600        0     0.31125   3.34901   0.46072  H
 C-CT-0.065100        0    -0.36775   1.98213   0.22081  H
 C-CT--0.090300       0    -0.41534   1.04542   1.44149  H
 C-C-0.735400         0    -1.46831  -0.05309   1.27325  H
 O-O--0.613300        0    -1.20679  -1.23572   1.15085  H
 N-N--1.003100        0    -2.76261   0.41228   1.16347  H
 C-C-0.612300         0     1.74457   3.43275  -0.11208  H
 O-O--0.571300        0     1.8529    3.437    -1.34566  H
 O-OS--0.421200       0     2.58084   2.36362   0.56742  H
 P-P-1.166200         0     3.91985   1.71308   0.01652  H
 O-O2--0.776000       0     4.96922   1.80903   1.19806  H
 O-O2--0.776000       0     4.48127   2.18394  -1.29256  H
 O-OS--0.498900       0     3.72254   0.13127  -0.04231  H
 C-CT-0.055800        0     3.0572   -0.35286  -1.22568  H
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 C-CT-0.106500        0     2.53142  -1.78815  -1.02607  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.53219  -2.72891  -0.63445  L
 C-CT-0.039400        0     3.39496  -2.99828   0.76109  L
 N-N*--0.025100       0     4.72363  -2.93147   1.4209   L
 C-CB-0.305300        0     5.48704  -4.03136   1.727    L
 N-NC--0.699700       0     5.13696  -5.3379    1.55956  L
 C-CQ-0.587500        0     6.09178  -6.16326   1.95344  L
 N-NC--0.761500       0     7.28416  -5.86712   2.45324  L
 C-CA-0.700900        0     7.60069  -4.57527   2.56053  L
 N-N2--0.901900       0     8.83528  -4.38281   2.98993  L
 C-CB-0.051500        0     6.67812  -3.55877   2.21023  L
 N-NB--0.607300       0     6.69124  -2.15799   2.22609  L
 C-CK-0.200600        0     5.49509  -1.84578   1.7804   L
 C-CT-0.067000        0     2.30924  -2.07715   1.32285  L
 O-OH--0.613900       0     1.57169  -2.67621   2.37316  L
 C-CT-0.202200        0     1.47167  -1.85717   0.05785  L
 O-OH--0.654100       0     0.58872  -2.94904  -0.18484  L
 H-H-0.199600         0    -1.64032   3.77134  -1.38792  H
 H-H-0.199600         0     0.19192   4.93259  -0.86927  H
 H-H-0.199600         0    -0.87446   5.06242   0.39222  H
 H-HP-0.101500        0     0.32299   3.56031   1.53745  H
 H-HC-0.005000        0     0.09113   1.48008  -0.63883  H
 H-HC-0.005000        0    -1.39772   2.18897  -0.07902  H
 H-HC-0.033100        0    -0.68245   1.63116   2.3327   H
 H-HC-0.033100        0     0.5468    0.57435   1.64156  H
 H-H-0.442900         0    -3.4808   -0.27405   1.34236  H
 H-H-0.442900         0    -2.94899   1.291     1.65767  H
 H-H1-0.067900        0     3.75466  -0.34209  -2.06831  H
 H-H1-0.067900        0     2.20834   0.28627  -1.47007  H
 H-H1-0.117400        0     2.07179  -2.09222  -1.96672  L
 H-H2-0.200700        0     3.00813  -4.012     0.87642  L
 H-H5-0.047300        0     5.86732  -7.21539   1.85533  L
 H-H-0.411500         0     9.21169  -3.44865   3.03787  L
 H-H-0.411500         0     9.41771  -5.21215   3.05187  L
 H-H5-0.155300        0     5.15869  -0.82194   1.66674  L
 H-H1-0.097200        0     2.72825  -1.12949   1.65841  L
 H-HO-0.418600        0     2.12345  -2.69206   3.18062  L
 H-H1-0.061500        0     0.92433  -0.91975   0.08882  L
 H-HO-0.437600        0    -0.17768  -2.7338    0.3835   L
 O-OW--0.834000       0    -10.28759  -2.09129   11.55476  L
 H-HW-0.417000        0    -10.60262  -1.24666   11.15202  L
 H-HW-0.417000        0    -10.56101  -2.74554   10.88732  L
 O-OW--0.834000       0    -10.2421  -3.84826   9.47896  L
 H-HW-0.417000        0    -10.50344  -3.20782   8.78959  L
 H-HW-0.417000        0    -9.61161  -4.41761   8.99684  L
 O-OW--0.834000       0    -10.70942  -1.95799   7.62312  L
 H-HW-0.417000        0    -11.50336  -1.55017   8.05426  L
 H-HW-0.417000        0    -10.07635  -1.23323   7.6685   L
 O-OW--0.834000       0     5.01841   4.37299   1.24286  H
 H-HW-0.417000        0     5.48232   4.97733   0.63386  H
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H-HW-0.417000        0     5.16784   2.8011    1.27971  H
O-OW--0.834000       0     6.15381   3.01159   3.50782  H
H-HW-0.417000        0     5.41323   2.41091   3.33043  H
H-HW-0.417000        0     5.72721   3.87667   3.34102  H
O-OW--0.834000       0     6.52176   2.24636  -5.64063  L
H-HW-0.417000        0     7.4438    2.06475  -5.90527  L
H-HW-0.417000        0     6.31725   3.07728  -6.09148  L
O-OW--0.834000       0     5.17641   6.16121   8.5993   L
H-HW-0.417000        0     4.75472   5.49284   8.0221   L
H-HW-0.417000        0     4.58088   6.17483   9.35589  L
O-OW--0.834000       0     7.81222   1.58395   5.35383  H
H-HW-0.417000        0     7.24637   2.07138   4.72379  H
H-HW-0.417000        0     7.14956   0.91418   5.67889  H
O-OW--0.834000       0     5.41696   8.14862   2.12691  H
H-HW-0.417000        0     4.55268   8.51996   1.85291  H
H-HW-0.417000        0     5.90548   8.29045   1.2982   H
O-OW--0.834000       0     4.1481    15.85546   4.35864  L
H-HW-0.417000        0     3.73189   15.1237   3.87561  L
H-HW-0.417000        0     3.42952   16.4772   4.47364  L
O-OW--0.834000       0    -4.3135    2.10429   5.55061  L
H-HW-0.417000        0    -4.12115   2.06449   6.49177  L
H-HW-0.417000        0    -4.82138   2.95805   5.49011  L
O-OW--0.834000       0     0.13325   1.91164   12.09796  L
H-HW-0.417000        0    -0.20434   1.73521   12.99921  L
H-HW-0.417000        0    -0.08849   2.83965   11.98764  L
O-OW--0.834000       0    -2.40397   9.80657   5.84287  L
H-HW-0.417000        0    -2.2033    8.89473   6.13444  L
H-HW-0.417000        0    -1.92488   9.89312   4.9837   L
O-OW--0.834000       0     1.84226   9.08527   6.95272  L
H-HW-0.417000        0     1.36786   8.37701   6.48418  L
H-HW-0.417000        0     1.23752   9.84928   6.83226  L
O-OW--0.834000       0    -4.9888    8.99787   5.58622  L
H-HW-0.417000        0    -4.88211   8.09991   5.95787  L
H-HW-0.417000        0    -4.11708   9.40504   5.74384  L
O-OW--0.834000       0    -2.35131   7.27974   6.95672  L
H-HW-0.417000        0    -3.22166   6.86666   6.75447  L
H-HW-0.417000        0    -2.01036   6.74455   7.68715  L
O-OW--0.834000       0     0.02374   10.96259   6.35044  L
H-HW-0.417000        0     0.14388   11.04095   5.38867  L
H-HW-0.417000        0    -0.91127   10.69984   6.40935  L
O-O2--0.818800       0     5.9       8.38041  -0.66128  H
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**IC**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.58519 | -11.63051 | -5.55345 | L |
| C-C-0.597200 | 0 | -11.90496 | -10.61186 | -6.43877 | L |
| O-O--0.567900 | 0 | -11.52278 | -10.95724 | -7.5479 | L |
| H-HC-0.112300 | 0 | -11.97652 | -11.79204 | -4.66666 | L |
| H-HC-0.112300 | 0 | -12.67732 | -12.56411 | -6.10632 | L |
| H-HC-0.112300 | 0 | -13.57369 | -11.26519 | -5.28406 | L |
| N-N--0.415700 | 0 | -11.7239 | -9.39148 | -5.92488 | L |
| C-CT--0.058100 | -1 | -10.86191 | -8.36118 | -6.52391 | L |
| C-C-0.597300 | 0 | -9.83418 | -7.84905 | -5.50906 | L |
| O-O--0.567900 | 0 | -10.10815 | -7.78103 | -4.30436 | L |
| C-CT--0.007400 | 0 | -11.66959 | -7.25534 | -7.19844 | L |
| C-CC-0.186800 | 0 | -11.07554 | -6.76769 | -8.49395 | L |
| N-NB--0.543200 | 0 | -11.48855 | -7.15787 | -9.76743 | L |
| C-CW--0.220700 | 0 | -10.19432 | -5.73563 | -8.60717 | L |
| C-CR-0.163500 | 0 | -10.89888 | -6.30257 | -10.61571 | L |
| N-NA--0.279500 | 0 | -10.11926 | -5.437 | -9.9488 | L |
| H-H-0.271900 | 0 | -12.09155 | -9.19434 | -5.01007 | L |
| H-H1-0.136000 | 0 | -10.29544 | -8.84777 | -7.31999 | L |
| H-HC-0.036700 | 0 | -11.72494 | -6.40985 | -6.52255 | L |
| H-HC-0.036700 | 0 | -12.68177 | -7.60546 | -7.40578 | L |
| H-H4-0.186200 | 0 | -9.75378 | -5.17324 | -7.79928 | L |
| H-H-0.333900 | 0 | -9.76104 | -4.55988 | -10.34659 | L |
| H-H5-0.143500 | 0 | -11.08726 | -6.26215 | -11.67911 | L |
| N-N--0.415700 | 0 | -8.64184 | -7.51395 | -5.99621 | L |
| C-CT--0.038900 | -1 | -7.4838 | -7.0126 | -5.23475 | L |
| C-C-0.597300 | 0 | -6.71004 | -5.93061 | -6.02398 | L |
| O-O--0.567900 | 0 | -7.06151 | -5.61227 | -7.15956 | L |
| C-CT-0.365400 | 0 | -6.49496 | -8.1445 | -4.88381 | L |
| O-OH--0.676100 | 0 | -6.21252 | -8.92197 | -6.00861 | L |
| C-CT--0.243800 | -1 | -7.0068 | -9.09244 | -3.81785 | L |
| H-H-0.271900 | 0 | -8.48824 | -7.70683 | -6.98008 | L |
| H-H1-0.100700 | 0 | -7.8172 | -6.57947 | -4.29877 | L |
| H-H1-0.004300 | 0 | -5.56428 | -7.71603 | -4.5119 | L |
| H-HC-0.064200 | 0 | -7.28104 | -8.53035 | -2.92505 | L |
| H-HC-0.064200 | 0 | -6.22812 | -9.80895 | -3.56098 | L |
| H-HC-0.064200 | 0 | -7.88255 | -9.62688 | -4.18695 | L |
| H-HO-0.410200 | 0 | -5.4987 | -9.54706 | -5.8026 | L |
| N-N--0.347900 | 0 | -5.63042 | -5.35831 | -5.45438 | L |
| C-CT--0.263700 | -1 | -4.64958 | -4.50242 | -6.17057 | L |
| C-C-0.734100 | 0 | -3.24567 | -4.56177 | -5.57986 | L |
| O-O--0.589400 | 0 | -3.12945 | -4.77828 | -4.37913 | L |
| C-CT--0.000700 | 0 | -5.16972 | -3.04979 | -6.28442 | L |
| C-CT-0.039000 | 0 | -4.98577 | -2.10459 | -5.07832 | L |
| C-CT-0.048600 | 0 | -5.75778 | -2.42521 | -3.79369 | L |
| N-N2--0.529500 | 0 | -5.13368 | -3.48442 | -2.99122 | L |
| C-CA-0.807600 | 0 | -5.075 | -3.5681 | -1.68046 | L |
| N-N2--0.862700 | 0 | -5.72386 | -2.78617 | -0.87179 | L |
| N-N2--0.862700 | 0 | -4.31589 | -4.47822 | -1.15642 | L |
| H-H-0.274700 | 0 | -5.3923 | -5.67163 | -4.52552 | L |
| H-H1-0.156000 | 0 | -4.58718 | -4.90726 | -7.17672 | L |

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 H-HC-0.032700        0    -6.22545  -3.06438  -6.5588   L
 H-HC-0.032700        0    -4.64493  -2.58758  -7.12211  L
 H-HC-0.028500        0    -5.33858  -1.12478  -5.3924   L
 H-HC-0.028500        0    -3.927    -2.00321  -4.84956  L
 H-H1-0.068700        0    -6.7829   -2.68705  -4.04852  L
 H-H1-0.068700        0    -5.76976  -1.51231  -3.19735  L
 H-H-0.345600         0    -4.50099  -4.10338  -3.47525  L
 H-H-0.447800         0    -5.74254  -2.92027   0.12758  L
 H-H-0.447800         0    -6.43586  -2.15068  -1.25665  L
 H-H-0.447800         0    -4.01363  -4.34577  -0.19756  L
 H-H-0.447800         0    -3.88944  -5.18386  -1.74929  L
 N-N--0.415700        0    -2.18812  -4.28518  -6.33999  L
 C-CT--0.002400      -1    -0.95493  -3.74257  -5.74163  L
 C-C-0.597300         0    -1.12936  -2.21306  -5.56713  L
 O-O--0.567900        0    -1.40118  -1.55851  -6.5747   L
 C-CT--0.034300       0     0.27148  -4.08147  -6.59558  L
 C-CA-0.011800        0     1.56828  -3.51472  -6.03735  L
 C-CA--0.125600       0     2.01357  -3.86972  -4.74664  L
 C-CA--0.125600       0     2.32978  -2.6149   -6.80524  L
 C-CA--0.170400       0     3.19404  -3.30517  -4.22717  L
 C-CA--0.170400       0     3.51053  -2.05659  -6.28995  L
 C-CA--0.107200       0     3.93142  -2.38511  -4.99279  L
 H-H-0.271900         0    -2.38088  -4.13075  -7.32559  L
 H-H1-0.097800        0    -0.79254  -4.21244  -4.77497  L
 H-HC-0.029500        0     0.11367  -3.70697  -7.60855  L
 H-HC-0.029500        0     0.36933  -5.16604  -6.64768  L
 H-HA-0.133000        0     1.44701  -4.56636  -4.14534  L
 H-HA-0.133000        0     2.00217  -2.33041  -7.79099  L
 H-HA-0.143000        0     3.53109  -3.56471  -3.23477  L
 H-HA-0.143000        0     4.07655  -1.34901  -6.87993  L
 H-HA-0.129700        0     4.81575  -1.91217  -4.59091  L
 N-N--0.254800        0    -1.05812  -1.65236  -4.33684  L
 C-CT--0.026600       0    -1.2818   -0.22666  -4.05074  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.02968   0.52437  -3.66839  H
 O-O--0.574800        0     0.56568   0.33566  -2.58911  H
 C-CT--0.007000       0    -2.25225  -0.27463  -2.86587  L
 C-CT-0.018900        0    -1.78083  -1.47497  -2.05038  L
 C-CT-0.019200        0    -1.1207   -2.39359  -3.07744  L
 H-H1-0.064100        0    -1.77211   0.28583  -4.87376  L
 H-HC-0.025300        0    -3.26642  -0.44727  -3.22457  L
 H-HC-0.025300        0    -2.21663   0.62407  -2.26131  L
 H-HC-0.021300        0    -2.61531  -1.96328  -1.54787  L
 H-HC-0.021300        0    -1.04398  -1.15369  -1.31974  L
 H-H1-0.039100        0    -0.1178   -2.66523  -2.74892  L
 H-H1-0.039100        0    -1.7328   -3.28486  -3.16698  L
 N-N--0.254800        0     0.54661   1.43856  -4.55115  H
 C-CT--0.026600       0     1.86779   2.00811  -4.28816  H
 C-C-0.589600         0     1.97671   3.50461  -4.63213  H
 O-O--0.574800        0     1.51338   3.95326  -5.6694   H
 C-CT--0.007000       0     2.73526   1.28358  -5.33864  H
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 C-CT-0.018900        0     1.81676   1.22929  -6.57569  H
 C-CT-0.019200        0     0.3809    1.36135  -6.00622  H
 H-H1-0.064100        0     2.15443   1.82771  -3.25303  H
 H-HC-0.025300        0     2.95495   0.28488  -4.95594  H
 H-HC-0.025300        0     3.68347   1.79425  -5.5349   H
 H-HC-0.021300        0     1.9457    0.30009  -7.13301  H
 H-HC-0.021300        0     2.02299   2.06306  -7.24741  H
 H-H1-0.039100        0    -0.10153   2.27177  -6.34586  H
 H-H1-0.039100        0    -0.23748   0.51295  -6.28714  H
 N-N--0.415700        0     2.76625   4.17599  -3.73654  H
 C-CT-0.039700        0     3.23066   5.56006  -3.89158  H
 C-C-0.597300         0     4.15462   5.6673   -5.1592   L    H-H1
111   0.        0.
 O-O--0.567900        0     5.19611   5.00137  -5.17475  L
 C-CT--0.003600       0     3.83408   5.88752  -2.48214  H
 C-CT-0.013600        0     5.03363   6.81622  -2.32134  H
 C-C-0.805400         0     5.61127   6.74812  -0.90864  H
 O-O2--0.818800       0     5.87176   5.6918   -0.34294  H
 H-H-0.271900         0     2.60002   3.89006  -2.76268  H
 H-H1-0.110500        0     2.39832   6.25494  -4.06067  H
 H-HC--0.017300       0     3.01141   6.25894  -1.87586  H
 H-HC--0.017300       0     4.07656   4.9557   -1.96191  H
 H-HC--0.042500       0     4.81669   7.85573  -2.57259  H
 H-HC--0.042500       0     5.85726   6.50136  -2.97384  H
 N-N--0.254800        0     3.80175   6.40173  -6.25702  L
 C-CT--0.026600       -1    4.65506   6.65762  -7.4558   L
 C-C-0.589600         0     6.09104   7.09945  -7.12565  L
 O-O--0.574800        0     6.99159   6.90568  -7.94405  L
 C-CT--0.007000       0     3.90868   7.66049  -8.3207   L
 C-CT-0.018900        0     2.45068   7.44795  -7.93728  L
 C-CT-0.019200        0     2.49579   7.02228  -6.4699   L
 H-H1-0.064100        0     4.71954   5.72409  -8.01088  L
 H-HC-0.025300        0     4.07854   7.48703  -9.38373  L
 H-HC-0.025300        0     4.21296   8.66007  -8.04619  L
 H-HC-0.021300        0     2.02871   6.64271  -8.53721  L
 H-HC-0.021300        0     1.8838    8.36527  -8.07473  L
 H-H1-0.039100        0     2.38116   7.89527  -5.83151  L
 H-H1-0.039100        0     1.68175   6.3295   -6.26808  L
 N-N--0.415700        0     6.34419   7.66102  -5.93736  L
 C-CT-0.014300        -1    7.68971   7.86659  -5.41762  L
 C-C-0.597300         0     8.49158   6.57202  -5.29504  L
 O-O--0.567900        0     8.33342   5.77878  -4.36539  L
 C-CT--0.204100       0     7.699     8.64269  -4.08307  L
 C-C-0.713000         0     9.10994   8.98953  -3.62438  L
 O-O--0.593100        0     9.72537   8.34048  -2.78932  L
 N-N--0.919100        0     9.69666   10.02866  -4.16304  L
 H-H-0.271900         0     5.54005   7.91924  -5.36335  L
 H-H1-0.104800        0     8.20316   8.50037  -6.14244  L
 H-HC-0.079700        0     7.24621   8.05164  -3.29828  L
 H-HC-0.079700        0     7.12573   9.55614  -4.18904  L
 H-H-0.419600         0     10.61018   10.2481  -3.81966  L
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H-H-0.419600          0     9.20018   10.6347  -4.81393  L
N-N--0.415700         0     9.45529   6.43778  -6.19621  L
C-CT--0.025200        -1    10.68061   5.72367  -5.91611  L
C-C-0.597300          0     11.04408   4.71032  -7.00679  L
O-O--0.567900         0     11.55594   5.06144  -8.06581  L
H-H-0.271900          0     9.40836   7.02835  -7.01457  L
H-H1-0.069800         0     10.62145   5.21082  -4.95553  L
H-H1-0.069800         0     11.49386   6.4462   -5.85306  L
N-N--0.415700         0     10.79552   3.44127  -6.70194  L
C-CT--0.001400        -1    10.81061   2.25717  -7.57339  L
C-C-0.597300          0     9.73489   1.3242   -6.98399  L
O-O--0.567900         0     8.88001   1.77308  -6.21075  L
C-CT--0.015200        0     12.23723   1.66827  -7.61894  L
C-CA--0.001100        0     12.67309   1.2631   -9.01329  L
C-CA--0.190600        0     13.039    2.26579  -9.93283  L
C-CA--0.190600        0     12.71359  -0.09152  -9.39789  L
C-CA--0.234100        0     13.44303   1.92099  -11.23678  L
C-CA--0.234100        0     13.10988  -0.44027  -10.7036  L
C-C-0.322600          0     13.47424   0.5637   -11.62413  L
O-OH--0.557900        0     13.85469   0.22273  -12.88296  L
H-H-0.271900          0     10.28049   3.3097   -5.84281  L
H-H1-0.087600         0     10.5018   2.55119  -8.57758  L
H-HC-0.029500         0     12.32908   0.82471  -6.93418  L
H-HC-0.029500         0     12.94872   2.42042  -7.27363  L
H-HA-0.169900         0     12.99618   3.3061   -9.63266  L
H-HA-0.169900         0     12.4416  -0.86998  -8.70031  L
H-HA-0.165600         0     13.71728   2.69602  -11.93481  L
H-HA-0.165600         0     13.13549  -1.47292  -11.01609  L
H-HO-0.399200         0     14.06621   0.99793  -13.40255  L
N-N--0.415700         0     9.83052   0.02272  -7.20878  L
C-CT--0.051800        -1    9.38893  -0.96637  -6.22553  L
C-C-0.597300          0     10.5623  -1.87271  -5.89968  L
O-O--0.567900         0     11.5428  -1.96237  -6.63841  L
C-CT--0.110200        0     8.13054  -1.6917   -6.74726  L
C-CT-0.353100         0     8.32809  -2.59893  -7.98158  L
C-CT--0.412100        0     8.73155  -4.02819  -7.59789  L
C-CT--0.412100        0     7.01551  -2.69136  -8.75806  L
H-H-0.271900          0     10.49662  -0.27428  -7.90919  L
H-H1-0.092200         0     9.12264  -0.4478   -5.30738  L
H-HC-0.045700         0     7.40059  -0.91737  -6.99043  L
H-HC-0.045700         0     7.69691  -2.28522  -5.94368  L
H-HC--0.036100        0     9.0848   -2.17778  -8.64312  L
H-HC-0.100000         0     9.71823  -4.03687  -7.14218  L
H-HC-0.100000         0     8.77115  -4.64699  -8.49425  L
H-HC-0.100000         0     8.00694  -4.45133  -6.9029   L
H-HC-0.100000         0     6.21649  -3.056    -8.1178   L
H-HC-0.100000         0     7.13103  -3.34818  -9.62061  L
H-HC-0.100000         0     6.74505  -1.704    -9.11759  L
N-N--0.415700         0     10.47728  -2.52223  -4.75463  L
C-CT--0.058100        -1    11.56116  -3.32073  -4.20214  L
C-C-0.597300          0     11.05804  -4.71516  -3.85407  L
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 O-O--0.567900        0     9.85974  -4.98765  -3.85824  L
 C-CT--0.007400       0     12.13865  -2.57007  -2.98783  L
 C-CC-0.186800        0     11.11874  -2.22402  -1.92417  L
 N-NB--0.543200       0     10.72362  -3.04916  -0.87111  L
 C-CW--0.220700       0     10.38357  -1.07608  -1.88214  L
 C-CR-0.163500        0     9.76761  -2.37335  -0.21057  L
 N-NA--0.279500       0     9.52997  -1.19486  -0.80674  L
 H-H-0.271900         0     9.61852  -2.41838  -4.22715  L
 H-H1-0.136000        0     12.35262  -3.44052  -4.94408  L
 H-HC-0.036700        0     12.59016  -1.64158  -3.34029  L
 H-HC-0.036700        0     12.9336  -3.16324  -2.54162  L
 H-H4-0.186200        0     10.4245  -0.2663   -2.59809  L
 H-H-0.333900         0     8.77032  -0.56821  -0.56726  L
 H-H5-0.143500        0     9.22335  -2.74029   0.6506   L
 N-N--0.415700        0     11.96957  -5.63271  -3.54877  L
 C-CT--0.059700       -1    11.57524  -7.00729  -3.23887  L
 C-C-0.597300         0     10.65575  -7.13257  -1.99839  L
 O-O--0.567900        0     9.88994  -8.08862  -1.89226  L
 C-CT-0.130300        0     12.80764  -7.9229   -3.14292  L
 C-CT--0.043000       0     12.34427  -9.39238  -3.05862  L
 C-CT--0.320400       0     13.73476  -7.54422  -1.97271  L
 C-CT--0.066000       -1    13.4046  -10.37387  -3.53677  L
 H-H-0.271900         0     12.94706  -5.38859  -3.57968  L
 H-H1-0.086900        0     10.99109  -7.35951  -4.08669  L
 H-HC-0.018700        0     13.36933  -7.79882  -4.07095  L
 H-HC-0.023600        0     11.47099  -9.53716  -3.69549  L
 H-HC-0.023600        0     12.06545  -9.64163  -2.0339   L
 H-HC-0.088200        0     14.6353  -8.15418  -2.008    L
 H-HC-0.088200        0     13.23702  -7.70826  -1.01629  L
 H-HC-0.088200        0     14.03928  -6.50104  -2.04211  L
 H-HC-0.018600        0     13.0068  -11.38773  -3.48456  L
 H-HC-0.018600        0     14.29025  -10.31205  -2.90478  L
 H-HC-0.018600        0     13.67864  -10.15466  -4.56934  L
 N-N--0.415700        0     10.67384  -6.16021  -1.07979  L
 C-CT--0.025200       -1    9.65117  -6.02674  -0.04103  L
 C-C-0.597300         0     8.25512  -5.89898  -0.65004  L
 O-O--0.567900        0     7.43392  -6.80785  -0.51278  L
 H-H-0.271900         0     11.29495  -5.3772   -1.22069  L
 H-H1-0.069800        0     9.86106  -5.15775   0.57821  L
 H-H1-0.069800        0     9.6664   -6.9122    0.58976  L
 N-N--0.415700        0     8.01306  -4.80931  -1.39055  L
 C-CT--0.058100       0     6.81696  -4.62264  -2.22782  L    H-HC
246   0.        0.
 C-C-0.597300         0     6.46557  -5.88947  -3.03201  L
 O-O--0.567900        0     5.2934   -6.25223  -3.1016   L
 C-CT--0.007400       0     6.99882  -3.4394   -3.18731  H
 C-CC-0.186800        0     6.9345   -2.01912  -2.7089   H
 N-NB--0.543200       0     7.57671  -1.08617  -3.48804  H
 C-CW--0.220700       0     6.18753  -1.38021  -1.75149  H
 C-CR-0.163500        0     7.17196   0.08359  -3.05223  H
 N-NA--0.279500       0     6.34532  -0.03186  -1.97979  H
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H-H-0.271900          0     8.78008  -4.15703  -1.50367  L
H-H1-0.136000         0     5.95883  -4.41369  -1.58593  L
H-HC-0.036700         0     6.23012  -3.54791  -3.96047  H
H-HC-0.036700         0     7.94143  -3.55029  -3.71762  H
H-H4-0.186200         0     5.54741  -1.71869  -0.95999  H
H-H-0.333900          0     5.77167   0.72304  -1.59184  H
H-H5-0.143500         0     7.46017   1.04802  -3.46358  H
N-N--0.415700         0     7.45566  -6.59227  -3.60078  L
C-CT-0.033700         -1    7.26198  -7.84875  -4.33352  L
C-C-0.597300          0     6.45296  -8.9146   -3.59058  L
O-O--0.567900         0     5.62361  -9.5789   -4.2116   L
C-CT--0.182500        0     8.57773  -8.384    -4.90297  L
H-H-0.271900          0     8.3856   -6.19099  -3.55086  L
H-H1-0.082300         0     6.65302  -7.5889   -5.19792  L
H-HC-0.060300         0     9.12741  -7.57828  -5.39084  L
H-HC-0.060300         0     8.35826  -9.15362  -5.64423  L
H-HC-0.060300         0     9.17775  -8.83421  -4.11774  L
N-N--0.347900         0     6.62408  -9.06437  -2.27253  L
C-CT--0.240000        -1    5.73821  -9.92694  -1.4798   L
C-C-0.734100          0     4.26365  -9.46939  -1.53465  L
O-O--0.589400         0     3.38626  -10.31369  -1.69411  L
C-CT--0.009400        0     6.25512  -10.06813  -0.03808  L
C-CT-0.018700         0     5.3738   -11.02387   0.79187  L
C-CT--0.047900        0     6.00145  -11.3284   2.15607  L
C-CT--0.014300        0     5.03783  -12.10399   3.06234  L
N-N3--0.385400        0     5.6217   -12.31486   4.41189  L
H-H-0.274700          0     7.30572  -8.46004  -1.81863  L
H-H1-0.142600         0     5.75151  -10.91852  -1.93576  L
H-HC-0.036200         0     6.27733  -9.08896   0.44133  L
H-HC-0.036200         0     7.27336  -10.45947  -0.07349  L
H-HC-0.010300         0     5.23604  -11.96028   0.24881  L
H-HC-0.010300         0     4.39844  -10.56265   0.95098  L
H-HC-0.062100         0     6.24843  -10.38166   2.63464  L
H-HC-0.062100         0     6.91188  -11.91071   2.00683  L
H-HP-0.113500         0     4.78025  -13.05875   2.59508  L
H-HP-0.113500         0     4.12009  -11.51354   3.15932  L
H-H-0.340000          0     4.90269  -12.57541   5.08278  L
H-H-0.340000          0     5.98026  -11.42654   4.76304  L
H-H-0.340000          0     6.37121  -12.98825   4.40989  L
N-N--0.415700         0     3.98008  -8.16759  -1.40052  L
C-CT--0.024900        -1    2.62859  -7.58947  -1.57126  L
C-C-0.597300          0     2.0724   -7.85491  -2.98071  L
O-O--0.567900         0     0.94676  -8.33646  -3.08008  L
C-CT-0.211700         0     2.61427  -6.0857   -1.24325  L
O-OH--0.654600        0     1.27526  -5.63824  -1.14615  L
H-H-0.271900          0     4.76952  -7.53662  -1.35519  L
H-H1-0.084300         0     1.96015  -8.0833   -0.86519  L
H-H1-0.035200         0     3.13386  -5.52245  -2.01738  L
H-H1-0.035200         0     3.11346  -5.9224   -0.28832  L
H-HO-0.427500         0     1.23696  -4.71141  -0.83809  L
N-N--0.415700         0     2.84676  -7.62366  -4.05794  L
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C-CT--0.059700       -1    2.51692  -8.0419   -5.4475   L
C-C-0.597300         0     2.10188  -9.53099  -5.43365  L
O-O--0.567900        0     0.97549  -9.84638  -5.79737  L
C-CT-0.130300        0     3.66515  -7.74082  -6.44002  L
C-CT--0.043000       0     3.9877   -6.23054  -6.4481   L
C-CT--0.320400       0     3.29371  -8.20459  -7.86075  L
C-CT--0.066000       0     5.21772  -5.8468   -7.27461  L
H-H-0.271900         0     3.74732  -7.18975  -3.88157  L
H-H1-0.086900        0     1.64301  -7.47405  -5.76959  L
H-HC-0.018700        0     4.55356  -8.28599  -6.1274   L
H-HC-0.023600        0     4.17584  -5.89284  -5.4314   L
H-HC-0.023600        0     3.12764  -5.68066  -6.8292   L
H-HC-0.088200        0     2.4425   -7.634    -8.23406  L
H-HC-0.088200        0     3.04423  -9.26567  -7.87452  L
H-HC-0.088200        0     4.1352   -8.06019  -8.53769  L
H-HC-0.018600        0     4.99643  -5.9113   -8.33992  L
H-HC-0.018600        0     6.05825  -6.4965   -7.03589  L
H-HC-0.018600        0     5.48584  -4.82138  -7.03094  L
N-N--0.415700        0     2.96076  -10.44482  -4.96355  L
C-CT-0.021300        -1    2.7317   -11.9027  -4.97522  L
C-C-0.597300         0     1.5089   -12.40579  -4.20953  L
O-O--0.567900        0     0.95588  -13.44049  -4.56768  L
C-CT--0.123100       -1    4.03957  -12.64604  -4.56637  L
S-SH--0.311900       0     5.38477  -12.30254  -5.73748  L
H-H-0.271900         0     3.8654   -10.11063  -4.65472  L
H-H1-0.112400        0     2.53171  -12.18025  -6.01212  L
H-H1-0.111200        0     3.84273  -13.7201  -4.56722  L
H-H1-0.111200        0     4.33371  -12.34291  -3.56075  L
H-HS-0.193300        0     5.54733  -11.01078  -5.41396  L
N-N--0.415700        0     1.08412  -11.70196  -3.16474  L
C-CT--0.051800       -1   -0.14874  -12.01233  -2.44699  L
C-C-0.597300         0    -1.37873  -11.36296  -3.10764  L
O-O--0.567900        0    -2.35666  -12.06389  -3.34265  L
C-CT--0.110200       0     0.00098  -11.5458  -0.98762  L
C-CT-0.353100        0     1.01924  -12.37736  -0.18311  L
C-CT--0.412100       0     1.36772  -11.6556   1.11658  L
C-CT--0.412100       0     0.47644  -13.76176   0.17883  L
H-H-0.271900         0     1.62739  -10.88894  -2.90178  L
H-H1-0.092200        0    -0.3225   -13.08907  -2.45979  L
H-HC-0.045700        0    -0.96956  -11.60584  -0.4928   L
H-HC-0.045700        0     0.30929  -10.49849  -0.98838  L
H-HC--0.036100       0     1.93975  -12.50151  -0.7526   L
H-HC-0.100000        0     1.8159   -10.69411   0.87009  L
H-HC-0.100000        0     2.07673  -12.24582   1.69228  L
H-HC-0.100000        0     0.46377  -11.48704   1.70376  L
H-HC-0.100000        0     1.20967  -14.30649   0.77122  L
H-HC-0.100000        0     0.27843  -14.33186  -0.72851  L
H-HC-0.100000        0    -0.44991  -13.66497   0.74595  L
N-N--0.415700        0    -1.34963  -10.05975  -3.42895  L
C-CT-0.014300        -1   -2.44772  -9.36156  -4.12646  L
C-C-0.597300         0    -2.80895  -10.04511  -5.43071  L
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O-O--0.567900        0    -3.95885  -10.43767  -5.63181  L
C-CT--0.204100       0    -2.1705   -7.85873  -4.23819  L
C-C-0.713000         0    -2.38081  -7.16845  -2.89939  L
O-O--0.593100        0    -3.49188  -6.86254  -2.49142  L
N-N--0.919100        0    -1.33192  -6.90398  -2.16117  L
H-H-0.271900         0    -0.4935   -9.54864  -3.24796  L
H-H1-0.104800        0    -3.34148  -9.47052  -3.50694  L
H-HC-0.079700        0    -2.8827   -7.42672  -4.93954  L
H-HC-0.079700        0    -1.16575  -7.67512  -4.61635  L
H-H-0.419600         0    -1.46298  -6.39861  -1.30556  L
H-H-0.419600         0    -0.41099  -7.18426  -2.47077  L
N-N--0.415700        0    -1.79799  -10.27273  -6.2577   L
C-CT--0.002400       -1   -1.94279  -11.08974  -7.44104  L
C-C-0.597300         0    -2.13452  -12.58489  -7.20089  L
O-O--0.567900        0    -2.62002  -13.28932  -8.08046  L
C-CT--0.034300       0    -0.8089   -10.80204  -8.44094  L
C-CA-0.011800        0    -0.94127  -9.44963  -9.12581  L
C-CA--0.125600       0    -1.67504  -9.34432  -10.32344  L
C-CA--0.125600       0    -0.38929  -8.28762  -8.55153  L
C-CA--0.170400       0    -1.87058  -8.08995  -10.92935  L
C-CA--0.170400       0    -0.57545  -7.03398  -9.16383  L
C-CA--0.107200       0    -1.32436  -6.93354  -10.34823  L
H-H-0.271900         0    -0.87297  -9.93778  -6.01441  L
H-H1-0.097800        0    -2.86346  -10.77705  -7.93703  L
H-HC-0.029500        0    -0.82882  -11.56835  -9.2173   L
H-HC-0.029500        0     0.15864  -10.88108  -7.94818  L
H-HA-0.133000        0    -2.12003  -10.22375  -10.76661  L
H-HA-0.133000        0     0.15694  -8.35121  -7.62594  L
H-HA-0.143000        0    -2.46629  -8.00668  -11.82897  L
H-HA-0.143000        0    -0.16675  -6.13958  -8.72001  L
H-HA-0.129700        0    -1.49654  -5.96797  -10.80516  L
N-N--0.415700        0    -1.79867  -13.06149  -6.00831  L
C-CT--0.025200       -1   -2.01316  -14.43371  -5.58123  L
C-C-0.597300         0    -3.47385  -14.8456  -5.43456  L
O-O--0.567900        0    -3.83024  -15.97996  -5.7395   L
H-H-0.271900         0    -1.4283   -12.41504  -5.33057  L
H-H1-0.069800        0    -1.52388  -14.58519  -4.61993  L
H-H1-0.069800        0    -1.54776  -15.10431  -6.30402  L
N-N--0.415700        0    -4.30684  -13.93428  -4.93442  L
C-CT--0.059700       -1   -5.76705  -14.08953  -4.8686   L
C-C-0.597300         0    -6.4321   -14.0458  -6.24775  L
O-O--0.567900        0    -7.44615  -14.71024  -6.45527  L
C-CT-0.130300        0    -6.32171  -13.04396  -3.84523  L
C-CT--0.043000       0    -5.9933   -13.5348  -2.39484  L
C-CT--0.320400       -1   -7.83691  -12.71795  -3.99525  L
C-CT--0.066000       -1   -5.30958  -12.52907  -1.43865  L
H-H-0.271900         0    -3.8934   -13.05471  -4.64846  L
H-H1-0.086900        0    -5.99189  -15.08477  -4.4831   L
H-HC-0.018700        0    -5.78684  -12.10828  -4.01662  L
H-HC-0.023600        0    -5.33274  -14.40135  -2.44354  L
H-HC-0.023600        0    -6.91283  -13.8824  -1.92219  L
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H-HC-0.088200        0    -8.02327  -12.24008  -4.95916  L
H-HC-0.088200        0    -8.14807  -12.03275  -3.20679  L
H-HC-0.088200        0    -8.42431  -13.63482  -3.93498  L
H-HC-0.018600        0    -4.35725  -12.20789  -1.85108  L
H-HC-0.018600        0    -5.14115  -12.99985  -0.47     L
H-HC-0.018600        0    -5.95326  -11.65893  -1.30896  L
N-N--0.415700        0    -5.83955  -13.31121  -7.19229  L
C-CT--0.149000      -1    -6.24152  -13.30529  -8.58716  L
H-H-0.271900         0    -5.00204  -12.81698  -6.92723  L
H-H1-0.097600        0    -6.51886  -14.31399  -8.8988   L
H-H1-0.097600        0    -5.41656  -12.95228  -9.20721  L
H-H1-0.097600        0    -7.10217  -12.64472  -8.71409  L
C-CT--0.366200      -1    -8.67438  -10.16266  -10.74256  L
C-C-0.597200         0    -7.92098  -9.47975  -9.66726  L
O-O--0.567900        0    -8.27064  -9.50167  -8.49473  L
H-HC-0.112300        0    -8.03702  -10.88516  -11.24671  L
H-HC-0.112300        0    -9.05862  -9.42019  -11.44032  L
H-HC-0.112300        0    -9.51999  -10.67826  -10.28578  L
N-N--0.415700        0    -6.86046  -8.85804  -10.1264  L
C-CT-0.021300       -1    -6.06636  -7.98673  -9.31912  L
C-C-0.597300         0    -5.57396  -6.82936  -10.18699  L
O-O--0.567900        0    -4.97653  -7.08097  -11.23714  L
C-CT--0.123100       0    -4.86477  -8.77391  -8.77437  L
S-SH--0.311900       0    -3.78558  -7.68347  -7.78994  L
H-H-0.271900         0    -6.67824  -8.87204  -11.11701  L
H-H1-0.112400        0    -6.65313  -7.59931  -8.48725  L
H-H1-0.111200        0    -4.29746  -9.18808  -9.60724  L
H-H1-0.111200        0    -5.22583  -9.5978   -8.15848  L
H-HS-0.193300        0    -3.3058   -6.96888  -8.82127  L
N-N--0.415700        0    -5.78969  -5.58427  -9.75983  L
C-CT-0.014300       -1    -5.3293   -4.41798  -10.50894  L
C-C-0.597300         0    -3.94845  -3.87851  -10.03261  L
O-O--0.567900        0    -3.37753  -4.32765  -9.03443  L
C-CT--0.204100       0    -6.45016  -3.362    -10.58776  L
C-C-0.713000         0    -6.26587  -2.37471  -11.73892  L
O-O--0.593100        0    -5.43637  -2.55787  -12.62012  L
N-N--0.919100        0    -6.98257  -1.28533  -11.76842  L
H-H-0.271900         0    -6.31103  -5.45147  -8.89823  L
H-H1-0.104800        0    -5.16338  -4.74338  -11.53767  L
H-HC-0.079700        0    -6.52654  -2.81655  -9.64765  L
H-HC-0.079700        0    -7.3903   -3.87821  -10.76787  L
H-H-0.419600         0    -6.84802  -0.6695   -12.54113  L
H-H-0.419600         0    -7.77915  -1.15753  -11.12959  L
N-N--0.415700        0    -3.38366  -2.90394  -10.74826  L
C-CT--0.051800      -1    -2.26431  -2.05465  -10.33164  L
C-C-0.597300         0    -2.83497  -0.63757  -10.05071  L
O-O--0.567900        0    -3.1083    0.10332  -10.99396  L
C-CT--0.110200       0    -1.18443  -2.05504  -11.43202  L
C-CT-0.353100        0    -0.03238  -1.05511  -11.19995  L
C-CT--0.412100       0     0.72822  -1.34208  -9.90656  L
C-CT--0.412100       0     0.9692   -1.14928  -12.35371  L
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H-H-0.271900          0    -3.903    -2.60097  -11.56908  L
H-H1-0.092200         0    -1.82727  -2.43506  -9.40812  L
H-HC-0.045700         0    -1.66131  -1.80495  -12.38152  L
H-HC-0.045700         0    -0.77539  -3.06244  -11.51589  L
H-HC--0.036100        0    -0.41712  -0.03763  -11.16631  L
H-HC-0.100000         0     1.09033  -2.36886  -9.91038  L
H-HC-0.100000         0     0.07172  -1.17751  -9.05114  L
H-HC-0.100000         0     1.56314  -0.64843  -9.81514  L
H-HC-0.100000         0     1.379    -2.15708  -12.41467  L
H-HC-0.100000         0     1.77507  -0.43526  -12.19246  L
H-HC-0.100000         0     0.4628   -0.90467  -13.2874  L
N-N--0.347900         0    -3.04027  -0.26226  -8.77402  L
C-CT--0.263700        -1   -3.40622   1.11882  -8.35867  L
C-C-0.734100          0    -2.15412   2.00072  -8.4489   L
O-O--0.589400         0    -1.03669   1.50163  -8.58496  L
C-CT--0.000700        0    -4.06764   1.07428  -6.9784   L
C-CT-0.039000         0    -4.81764   2.36591  -6.62974  L
C-CT-0.048600         0    -5.63341   2.20602  -5.35214  L
N-N2--0.529500        0    -4.78126   2.0665   -4.16716  L
C-CA-0.807600         0    -5.22997   1.96465  -2.93754  L
N-N2--0.862700        0    -6.46191   1.68439  -2.66614  L
N-N2--0.862700        0    -4.45353   2.14736  -1.91964  L
H-H-0.274700          0    -2.68165  -0.88273  -8.05832  L
H-H1-0.156000         0    -4.12536   1.50616  -9.08335  L
H-HC-0.032700         0    -3.3198    0.85819  -6.21882  L
H-HC-0.032700         0    -4.7991    0.26779  -6.99644  L
H-HC-0.028500         0    -5.4994    2.61753  -7.44334  L
H-HC-0.028500         0    -4.1205    3.18858  -6.48572  L
H-H1-0.068700         0    -6.31433   1.35724  -5.44723  L
H-H1-0.068700         0    -6.21319   3.11751  -5.22711  L
H-H-0.345600          0    -3.80146   2.3356   -4.27272  L
H-H-0.447800          0    -6.75577   1.60676  -1.70246  L
H-H-0.447800          0    -7.01066   1.14602  -3.33667  L
H-H-0.447800          0    -4.84438   1.99525  -1.00253  L
H-H-0.447800          0    -3.47254   2.3713   -2.08625  L
N-N--0.415700         0    -2.34307   3.3079   -8.35361  L
C-CT--0.002400        -1   -1.29751   4.27422  -8.04953  L
C-C-0.597300          0    -1.79256   5.15363  -6.90009  L
O-O--0.567900         0    -2.93403   5.60549  -6.91576  L
C-CT--0.034300        0    -0.91835   5.06979  -9.30288  L
C-CA-0.011800         0    -0.15253   4.23492  -10.3146  L
C-CA--0.125600        0     1.22661   4.00849  -10.13993  L
C-CA--0.125600        0    -0.82339   3.63338  -11.3959  L
C-CA--0.170400        0     1.93453   3.205    -11.0519  L
C-CA--0.170400        0    -0.11859   2.82177  -12.30281  L
C-CA--0.107200        0     1.26163   2.61216  -12.13523  L
H-H-0.271900          0    -3.28638   3.64497  -8.23659  L
H-H1-0.097800         0    -0.40107   3.76018  -7.70895  L
H-HC-0.029500         0    -0.29278   5.91213  -9.0056   L
H-HC-0.029500         0    -1.81996   5.47868  -9.76227  L
H-HA-0.133000         0     1.73641   4.43917  -9.29102  L
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 H-HA-0.133000        0    -1.88835   3.77479  -11.51583  L
 H-HA-0.143000        0     2.98935   3.03768  -10.90645  L
 H-HA-0.143000        0    -0.65062   2.34848  -13.11583  L
 H-HA-0.129700        0     1.7947    1.98441  -12.83264  L
 N-N--0.516300        0    -0.95803   5.3379    -5.8794   L
 C-CT-0.038100        0    -1.34164   5.93971   -4.60179  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.64857   7.30741   -4.44756  L
 O-O--0.581900        0     0.16921   7.51882   -3.54568  L
 C-CT--0.030300       0    -1.04458   4.95793   -3.45163  H
 C-C-0.799400         0    -1.75883   3.60862   -3.49977  H
 O-O2--0.801400       0    -1.90142   3.01917   -2.30902  H
 O-O2--0.801400       0    -2.20586   3.03427   -4.46627  H
 H-H-0.293600         0    -0.05497   4.88202   -5.93101  L
 H-H1-0.088000        0    -2.4167    6.12886   -4.59648  L
 H-HC--0.012200       0    -1.33292   5.44032   -2.5122   H
 H-HC--0.012200       0     0.03146   4.7515    -3.39298  H
 N-N--0.516300        0    -0.98069   8.21836   -5.36652  L
 C-CT-0.038100        0    -0.31602   9.49384   -5.69007  L
 C-C-0.536600         0    -0.82448   10.70401   -4.88207  L
 O-O--0.581900        0    -0.62749   11.86163   -5.25371  L
 C-CT--0.030300       0    -0.48507   9.7433    -7.20361  L
 C-C-0.799400         0    -1.9039    10.14808   -7.63016  L
 O-O2--0.801400       0    -2.86487   9.62926   -7.01622  L
 O-O2--0.801400       0    -2.00973   10.91205   -8.61641  L
 H-H-0.293600         0    -1.76096   8.01427   -5.98836  L
 H-H1-0.088000        0     0.74647   9.39401   -5.4822   L
 H-HC--0.012200       0    -0.22608   8.83257   -7.74314  L
 H-HC--0.012200       0     0.21716   10.52198   -7.5076   L
 N-N--0.415700        0    -1.45876   10.43986   -3.73966  L
 C-CT--0.038900       -1   -2.19808   11.39687   -2.89785  L
 C-C-0.597300         0    -1.30823   12.57124   -2.36218  L
 O-O--0.567900        0    -1.86132   13.55257   -1.86634  L
 C-CT-0.365400        0    -2.88044   10.67345   -1.74588  L
 O-OH--0.676100       0    -2.02921   9.76609   -1.0757   L
 C-CT--0.243800       -1   -3.9973    9.86263   -2.37204  L
 H-H-0.271900         0    -1.51629   9.46369   -3.49155  L
 H-H1-0.100700        0    -2.96514   11.86884   -3.51128  L
 H-H1-0.004300        0    -3.29548   11.38705   -1.03476  L
 H-HC-0.064200        0    -4.68744   10.5246   -2.89348  L
 H-HC-0.064200        0    -4.52238   9.35366   -1.57058  L
 H-HC-0.064200        0    -3.60977   9.11607   -3.06538  L
 H-HO-0.410200        0    -1.80364   10.18872   -0.2111   L
 N-N--0.415700        0     0.0399    12.55779   -2.50463  L
 C-CT-0.014300        -1    0.9553    13.72835   -2.3703   L
 C-C-0.597300         0     1.90685   13.82516   -3.5927   L
 O-O--0.567900        0     3.05342   13.37656   -3.49626  L
 C-CT--0.204100       0     1.69798   13.71977   -1.02455  L
 C-C-0.713000         0     2.55417   14.97123   -0.84481  L
 O-O--0.593100        0     2.70893   15.82509   -1.70789  L
 N-N--0.919100        0     3.15228   15.14189    0.30634  L
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 H-H-0.271900         0     0.38547   11.76346  -3.02992  L
 H-H1-0.104800        0     0.3406    14.6268  -2.35873  L
 H-HC-0.079700        0     2.33706   12.84065  -0.96761  L
 H-HC-0.079700        0     0.96332   13.67308  -0.22097  L
 H-H-0.419600         0     3.6772    15.99118   0.38917  L
 H-H-0.419600         0     2.97048   14.5185   1.08048  L
 N-N--0.254800        0     1.50277   14.48982  -4.70112  L
 C-CT--0.026600       -1    2.24999   14.51254  -5.96988  L
 C-C-0.589600         0     3.62083   15.17582  -5.90811  L
 O-O--0.574800        0     4.44168   15.00786  -6.80763  L
 C-CT--0.007000       0     1.31503   15.14784  -7.00379  L
 C-CT-0.018900        0     0.34632   15.97202  -6.16102  L
 C-CT-0.019200        0     0.21954   15.1579  -4.87615  L
 H-H1-0.064100        0     2.41295   13.47741  -6.26902  L
 H-HC-0.025300        0     0.76221   14.35893  -7.51759  L
 H-HC-0.025300        0     1.84932   15.76547  -7.72687  L
 H-HC-0.021300        0    -0.61733   16.09556  -6.65622  L
 H-HC-0.021300        0     0.79185   16.94194  -5.93546  L
 H-H1-0.039100        0    -0.00885   15.82399  -4.0443   L
 H-H1-0.039100        0    -0.56843   14.41157  -4.98789  L
 N-N--0.415700        0     3.92291   15.92112  -4.84771  L
 C-CT--0.025200       -1    5.09728   16.78172  -4.81274  L
 C-C-0.597300         0     6.43898   16.13121  -4.48829  L
 O-O--0.567900        0     7.38469   16.79892  -4.07478  L
 H-H-0.271900         0     3.27202   15.92698  -4.07062  L
 H-H1-0.069800        0     4.92637   17.55447  -4.06365  L
 H-H1-0.069800        0     5.20091   17.28222  -5.77599  L
 N-N--0.347900        0     6.51879   14.82963  -4.72215  L
 C-CT--0.240000       -1    7.68673   13.9511  -4.63461  L
 C-C-0.734100         0     7.60701   12.87996  -5.75901  L
 O-O--0.589400        0     8.38019   11.92294  -5.73573  L
 C-CT--0.009400       0     7.70848   13.32256  -3.20762  L
 C-CT-0.018700        0     6.46876   12.43502  -3.00795  L    H-HC
590   0.        0.
 C-CT--0.047900       0     6.1936    11.6723  -1.71099  H
 C-CT--0.014300       0     4.92149   10.88457  -2.0447   H
 N-N3--0.385400       0     4.48837   9.93415  -1.00725  H
 H-H-0.274700         0     5.64046   14.43069  -5.03341  L
 H-H1-0.142600        0     8.59691   14.53144  -4.78731  L
 H-HC-0.036200        0     7.71381   14.11477  -2.45715  L
 H-HC-0.036200        0     8.60869   12.71907  -3.08553  L
 H-HC-0.010300        0     6.55431   11.66753  -3.75863  L
 H-HC-0.010300        0     5.58557   13.03918  -3.20363  L
 H-HC-0.062100        0     6.03331   12.3754  -0.89185  H
 H-HC-0.062100        0     7.02721   11.00816  -1.47988  H
 H-HP-0.113500        0     5.08395   10.2809  -2.94501  H
 H-HP-0.113500        0     4.10566   11.57786  -2.29391  H
 H-H-0.340000         0     3.56526   9.60169  -1.28991  H
 H-H-0.340000         0     4.3626    10.41228  -0.10948  H
 H-H-0.340000         0     5.41514   8.69542  -0.6767   H
 N-N--0.516300        0     6.6503    12.97932  -6.69686  L
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C-CT-0.039700        -1    6.1203    11.87056  -7.52279  L
C-C-0.536600         0     6.27345   12.1787  -9.04062  L
O-O--0.581900        0     6.01735   13.29599  -9.48086  L
C-CT-0.056000        0     4.68215   11.50493  -7.08497  L
C-CT-0.013600        0     4.73093   11.16398  -5.58753  L
C-C-0.805400         0     3.76301   10.13754  -4.99372  L
O-O2--0.818800       0     2.67339   10.51202  -4.52413  L
O-O2--0.818800       0     4.24123   8.99777  -4.78705  L
H-H-0.293600         0     6.10111   13.83073  -6.75472  L
H-H1-0.110500        0     6.73381   10.98817  -7.34084  L
H-HC--0.017300       0     4.33861   10.65829  -7.66168  L
H-HC--0.017300       0     4.00657   12.3385  -7.26335  L
H-HC--0.042500       0     4.65256   12.09819  -5.03717  L
H-HC--0.042500       0     5.71881   10.74606  -5.4088   L
N-N--0.415700        0     6.77576   11.21786  -9.8446   L
C-CT--0.149000       -1    7.14986   11.39665  -11.26596  L
H-H-0.271900         0     6.94492   10.31872  -9.42149  L
H-H1-0.097600        0     7.90434   12.1807  -11.34911  L
H-H1-0.097600        0     6.26894   11.70136  -11.83481  L
H-H1-0.097600        0     7.54107   10.46469  -11.67477  L
C-CT--0.366200       0     9.996     2.27719  -12.01594  L
C-C-0.597200         0     8.98386   1.43048  -11.282   L
O-O--0.567900        0     9.27955   0.93425  -10.20072  L
H-HC-0.112300        0     10.56022   2.8499   -11.28178  L
H-HC-0.112300        0     9.50078   2.96131  -12.70166  L
H-HC-0.112300        0     10.6721   1.61792  -12.55648  L
N-N--0.415700        0     7.7922    1.28014  -11.86699  L
C-CT--0.059700       -1    6.69357   0.46504  -11.32193  L
C-C-0.597300         0     6.03973  -0.38122  -12.4321  L
O-O--0.567900        0     6.46486  -1.51006  -12.65704  L
C-CT-0.130300        0     5.67842   1.31577  -10.49795  L
C-CT--0.043000       0     6.3681    2.12892  -9.37247  L
C-CT--0.320400       0     4.58082   0.42274  -9.87716  L
C-CT--0.066000       0     5.42959   3.03886  -8.56805  L
H-H-0.271900         0     7.67212   1.71338  -12.76728  L
H-H1-0.086900        0     7.13591  -0.25286  -10.63409  L
H-HC-0.018700        0     5.20077   2.0259   -11.17437  L
H-HC-0.023600        0     7.12075   2.78115  -9.81349  L
H-HC-0.023600        0     6.87214   1.44706  -8.68547  L
H-HC-0.088200        0     4.12163  -0.22904  -10.61876  L
H-HC-0.088200        0     3.78351   1.03799  -9.45862  L
H-HC-0.088200        0     5.00013  -0.192    -9.08164  L
H-HC-0.018600        0     4.75766   2.44731  -7.94647  L
H-HC-0.018600        0     4.84772   3.66473  -9.245    L
H-HC-0.018600        0     6.02521   3.6807   -7.91839  L
N-N--0.415700        0     5.02119   0.14335  -13.13107  L
C-CT--0.149000       -1    4.24477  -0.58643  -14.1366  L
H-H-0.271900         0     4.72119   1.07099  -12.87604  L
H-H1-0.097600        0     3.82478  -1.49113  -13.69164  L
H-H1-0.097600        0     4.89279  -0.87605  -14.96579  L
H-H1-0.097600        0     3.43097   0.03558  -14.51267  L
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C-CT--0.366200       -1   -5.04165   16.98023  -3.10875  L
C-C-0.597200         0    -5.61517   16.21236  -1.93097  L
O-O--0.567900        0    -5.4574    16.66011  -0.79804  L
H-HC-0.112300        0    -5.85039   17.38115  -3.71458  L
H-HC-0.112300        0    -4.41363   16.3127  -3.69772  L
H-HC-0.112300        0    -4.42971   17.79584  -2.72798  L
N-N--0.254800        0    -6.34032   15.10892  -2.17621  L
C-CT--0.026600       -1   -7.02665   14.35652  -1.13238  L
C-C-0.589600         0    -6.17176   13.24983  -0.51559  L
O-O--0.574800        0    -5.63969   12.37264  -1.1928   L
C-CT--0.007000       0    -8.23452   13.75217  -1.85836  L
C-CT-0.018900        0    -7.70329   13.46985  -3.26668  L
C-CT-0.019200        0    -6.7053    14.60611  -3.49688  L
H-H1-0.064100        0    -7.38051   15.0283  -0.34977  L
H-HC-0.025300        0    -9.0315    14.49504  -1.91476  L
H-HC-0.025300        0    -8.59991   12.84679  -1.37378  L
H-HC-0.021300        0    -8.50343   13.48151  -4.00711  L
H-HC-0.021300        0    -7.18322   12.51191  -3.29148  L
H-H1-0.039100        0    -5.82791   14.2323  -4.02731  L
H-H1-0.039100        0    -7.18559   15.3974  -4.07316  L
N-N--0.415700        0    -6.11191   13.28251   0.80788  L
C-CT--0.023700       -1   -5.25112   12.45192   1.63735  L
C-C-0.597300         0    -5.43907   10.92387   1.52497  L
O-O--0.567900        0    -6.53682   10.4412   1.23336  L
C-CT-0.034200        0    -5.49319   12.83159   3.11202  L
C-CT-0.001800        0    -5.04431   14.25026   3.49188  L
S-S--0.273700        0    -3.25812   14.49436   3.70174  L
C-CT--0.053600       -1   -2.96171   13.53303   5.21438  L
H-H-0.271900         0    -6.59321   14.04317   1.2544   L
H-H1-0.088000        0    -4.21102   12.6715   1.38464  L
H-HC-0.024100        0    -4.98      12.122    3.76096  L
H-HC-0.024100        0    -6.56081   12.74108   3.3193   L
H-H1-0.044000        0    -5.5242    14.51398   4.43447  L
H-H1-0.044000        0    -5.39982   14.9524   2.7378   L
H-H1-0.068400        0    -3.14673   12.4748   5.02585  L
H-H1-0.068400        0    -3.61527   13.88238   6.01289  L
H-H1-0.068400        0    -1.92174   13.64892   5.51923  L
N-N--0.415700        0    -4.3765    10.17306   1.85773  L
C-CT--0.001400       -1   -4.2574    8.72059   1.69168  L
C-C-0.597300         0    -5.49454   7.84553   1.9988   L
O-O--0.567900        0    -6.09147   7.34505   1.05062  L
C-CT--0.015200       0    -2.96184   8.14747   2.28654  L
C-CA--0.001100       0    -2.90903   6.63569   2.44287  L
C-CA--0.190600       0    -3.08344   5.77115   1.34147  L
C-CA--0.190600       0    -2.7569    6.09756   3.72917  L
C-CA--0.234100       0    -3.14741   4.37466   1.54856  L
C-CA--0.234100       0    -2.84451   4.71433   3.94165  L
C-C-0.322600         0    -3.05271   3.84823   2.85564  L
O-OH--0.557900       0    -3.18454   2.51528   3.07316  L
H-H-0.271900         0    -3.49885   10.65656   2.02623  L
H-H1-0.087600        0    -4.12886   8.59086   0.61695  L
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H-HC-0.029500        0    -2.79651   8.61179   3.25749  L
H-HC-0.029500        0    -2.14245   8.41231   1.62649  L
H-HA-0.169900        0    -3.24195   6.19555   0.35713  L
H-HA-0.169900        0    -2.64335   6.75768   4.57524  L
H-HA-0.165600        0    -3.34946   3.69735   0.73218  L
H-HA-0.165600        0    -2.81837   4.33368   4.95049  L
H-HO-0.399200        0    -3.50735   2.37074   3.98373  L
N-N--0.516300        0    -5.84844   7.55269   3.25725  L
C-CT-0.038100       -1    -6.80496   6.47879   3.62705  L
C-C-0.536600         0    -8.21186   6.69768   3.06753  L
O-O--0.581900        0    -8.87725   5.73545   2.69159  L
C-CT--0.030300       0    -6.85399   6.30282   5.15674  L
C-C-0.799400         0    -5.58865   5.63989   5.71692  L
O-O2--0.801400       0    -5.48982   4.39216   5.61297  L
O-O2--0.801400       0    -4.71339   6.3748    6.23921  L
H-H-0.293600         0    -5.34368   8.02802   4.00098  L
H-H1-0.088000        0    -6.43615   5.54054   3.21873  L
H-HC--0.012200       0    -7.70441   5.66806   5.40865  L
H-HC--0.012200       0    -7.01873   7.27005   5.63402  L
N-N--0.415700        0    -8.65116   7.95529   2.9749   L
C-CT--0.002400       0    -9.84702   8.34693   2.22761  L
C-C-0.597300         0    -9.75186   7.90061   0.76049  L
O-O--0.567900        0    -10.60615   7.16018   0.27299  L
C-CT--0.034300       0    -10.05172   9.86502   2.34688  L
C-CA-0.011800        0    -11.10934   10.40914   1.40437  L
C-CA--0.125600       0    -12.47557   10.23487   1.69439  L
C-CA--0.125600       0    -10.72484   11.03267   0.20151  L
C-CA--0.170400       0    -13.45211   10.68647   0.7879   L
C-CA--0.170400       0    -11.70034   11.48164  -0.70556  L
C-CA--0.107200       0    -13.06459   11.30926  -0.41219  L
H-H-0.271900         0    -7.99502   8.66721   3.26314  L
H-H1-0.097800        0    -10.71338   7.84465   2.65934  L
H-HC-0.029500        0    -9.10777   10.37133   2.13932  L
H-HC-0.029500        0    -10.33226   10.10387   3.37343  L
H-HA-0.133000        0    -12.77495   9.73478   2.60431  L
H-HA-0.133000        0    -9.67605   11.13993  -0.04263  L
H-HA-0.143000        0    -14.49969   10.53804   1.0064   L
H-HA-0.143000        0    -11.39503   11.93963  -1.63578  L
H-HA-0.129700        0    -13.81359   11.64203  -1.11638  L
N-N--0.415700        0    -8.717     8.34273   0.04888  L
C-CT--0.038900      -1    -8.53298   8.04891  -1.37638  L
C-C-0.597300         0    -8.36695   6.5697   -1.67503  L
O-O--0.567900        0    -9.02173   6.02316  -2.55924  L
C-CT-0.365400        0    -7.37971   8.87987  -1.95092  L
O-OH--0.676100       0    -7.62596   10.24678  -1.69361  L
C-CT--0.243800       0    -7.25031   8.73231  -3.46733  L
H-H-0.271900         0    -8.0379    8.95311   0.49342  L
H-H1-0.100700        0    -9.43755   8.36771  -1.89381  L
H-H1-0.004300        0    -6.45657   8.57448  -1.46475  L
H-HC-0.064200        0    -8.20071   8.9693   -3.94563  L
H-HC-0.064200        0    -6.95918   7.71433  -3.72538  L
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H-HC-0.064200        0    -6.48984   9.41353  -3.84632  L
H-HO-0.410200        0    -6.77406   10.69542  -1.57174  L
N-N--0.415700        0    -7.52257   5.91671  -0.88908  L
C-CT--0.058100       -1   -7.38328   4.47444  -0.7592   L
C-C-0.597300         0    -8.72759   3.77529  -0.61705  L
O-O--0.567900        0    -9.03749   2.9093   -1.43489  L
C-CT--0.007400       0    -6.44356   4.25168   0.43008  L
C-CC-0.186800        0    -6.35613   2.85294   0.957    L
N-NB--0.543200       0    -6.42297   1.69845   0.18891  L
C-CW--0.220700       0    -6.25755   2.51408   2.27066  L
C-CR-0.163500        0    -6.41138   0.67506   1.04745  L
N-NA--0.279500       0    -6.29025   1.14061   2.30029  L
H-H-0.271900         0    -7.05202   6.49143  -0.19625  L
H-H1-0.136000        0    -6.9166    4.08164  -1.66118  L
H-HC-0.036700        0    -6.78718   4.8714    1.25065  L
H-HC-0.036700        0    -5.44966   4.5878    0.14486  L
H-H4-0.186200        0    -6.20137   3.18856   3.11717  L
H-H-0.333900         0    -6.28034   0.54536   3.12661  L
H-H5-0.143500        0    -6.50841  -0.36628   0.76468  L
N-N--0.415700        0    -9.52987   4.15611   0.38302  L
C-CT-0.021300        -1   -10.82789   3.53132   0.59173  L
C-C-0.597300         0    -11.74275   3.58194  -0.60987  L
O-O--0.567900        0    -12.35653   2.58157  -0.97855  L
C-CT--0.123100       0    -11.4821   3.92268   1.93456  L
S-SH--0.311900       0    -12.57321   5.37241   1.86163  L
H-H-0.271900         0    -9.22605   4.87905   1.0275   L
H-H1-0.112400        0    -10.60785   2.46758   0.69396  L
H-H1-0.111200        0    -10.70961   4.08878   2.6846   L
H-H1-0.111200        0    -12.08211   3.07724   2.27481  L
H-HS-0.193300        0    -11.66553   6.21556   1.35041  L
N-N--0.415700        0    -11.78586   4.74643  -1.2353   L
C-CT--0.059700       -1   -12.60467   4.9731   -2.3982   L
C-C-0.597300         0    -12.11322   4.26658  -3.66262  L
O-O--0.567900        0    -12.92626   3.64375  -4.3443   L
C-CT-0.130300        0    -12.83163   6.49926  -2.57287  L
C-CT--0.043000       0    -14.16494   6.94471  -1.92196  L
C-CT--0.320400       -1   -12.7416   7.00817  -4.01723  L
C-CT--0.066000       -1   -15.45671   6.5458   -2.6664   L
H-H-0.271900         0    -11.24173   5.50804  -0.84366  L
H-H1-0.086900        0    -13.57487   4.52212  -2.19253  L
H-HC-0.018700        0    -12.03619   7.02029  -2.03615  L
H-HC-0.023600        0    -14.15404   8.0317   -1.83005  L
H-HC-0.023600        0    -14.20845   6.53841  -0.9102   L
H-HC-0.088200        0    -11.72269   6.8983   -4.39028  L
H-HC-0.088200        0    -12.99293   8.0684   -4.04908  L
H-HC-0.088200        0    -13.42527   6.45925  -4.66633  L
H-HC-0.018600        0    -16.31968   6.85385  -2.07585  L
H-HC-0.018600        0    -15.49672   5.46613  -2.80996  L
H-HC-0.018600        0    -15.50454   7.04196  -3.63555  L
N-N--0.415700        0    -10.82129   4.35567  -3.99555  L
C-CT--0.024900       -1   -10.25242   3.62802  -5.13523  L
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C-C-0.597300          0    -10.51984   2.11714  -4.96747  L
O-O--0.567900         0    -10.93243   1.48367  -5.93156  L
C-CT-0.211700         0    -8.76381    3.89421  -5.29078  L
O-OH--0.654600        0    -8.32565    3.334    -6.51577  L
H-H-0.271900          0    -10.21012   4.89691  -3.39181  L
H-H1-0.084300         0    -10.75781   3.96038  -6.0427   L
H-H1-0.035200         0    -8.22757    3.44736  -4.45247  L
H-H1-0.035200         0    -8.57908    4.96949  -5.30106  L
H-HO-0.427500         0    -8.8863     2.57983  -6.74691  L
N-N--0.516300         0    -10.31743   1.53808  -3.77222  L
C-CT-0.038100         -1   -10.56686   0.10842  -3.49319  L
C-C-0.536600          0    -12.04629  -0.29431  -3.59762  L
O-O--0.581900         0    -12.38145  -1.25036  -4.30224  L
C-CT--0.030300        0    -9.94833   -0.31648  -2.15018  L
C-C-0.799400          0    -8.47067   -0.68662  -2.29663  L
O-O2--0.801400        0    -7.88196   -0.44587  -3.37505  L
O-O2--0.801400        0    -7.88533   -1.23217  -1.33391  L
H-H-0.293600          0    -9.96756    2.11277  -3.01212  L
H-H1-0.088000         0    -10.0778   -0.4596   -4.28336  L
H-HC--0.012200        0    -10.47607  -1.19282  -1.7735   L
H-HC--0.012200        0    -10.06763   0.47721  -1.41211  L
N-N--0.415700         0    -12.93386   0.43646  -2.91871  L
C-CT-0.033700         -1   -14.38827   0.31261  -3.03865  L
C-C-0.597300          0    -14.8616    0.3302   -4.50379  L
O-O--0.567900         0    -15.68678  -0.48988  -4.90183  L
C-CT--0.182500        -1   -14.99604   1.47251  -2.30938  L
H-H-0.271900          0    -12.57616   1.2001   -2.35344  L
H-H1-0.082300         0    -14.71443  -0.62375  -2.5851   L
H-HC-0.060300         0    -14.72953   1.42409  -1.25308  L
H-HC-0.060300         0    -16.0828    1.42582  -2.39129  L
H-HC-0.060300         0    -14.64895   2.41889  -2.72334  L
N-N--0.415700         0    -14.37237   1.3056   -5.27618  L
C-CT--0.025200        -1   -14.74787   1.55779  -6.66372  L
C-C-0.597300          0    -14.26221   0.49592  -7.64661  L
O-O--0.567900         0    -15.00677   0.09227  -8.53477  L
H-H-0.271900          0    -13.71165   1.94585  -4.84718  L
H-H1-0.069800         0    -14.33557   2.51728  -6.97344  L
H-H1-0.069800         0    -15.83413   1.60995  -6.7348   L
N-N--0.516300         0    -13.01032   0.07006  -7.49554  L
C-CT-0.039700         -1   -12.37894  -1.02022  -8.24389  L
C-C-0.536600          0    -13.11136  -2.36432  -8.07081  L
O-O--0.581900         0    -13.24857  -3.12303  -9.02712  L
C-CT-0.056000         0    -10.91429  -1.08065  -7.78273  L
C-CT-0.013600         0    -10.04018  -2.17183  -8.41013  L
C-C-0.805400          0    -9.60792   -1.88132  -9.84937  L
O-O2--0.818800        0    -9.60772   -2.82325  -10.67315  L
O-O2--0.818800        0    -9.11961   -0.76033  -10.10872  L
H-H-0.293600          0    -12.44571   0.51157  -6.77632  L
H-H1-0.110500         0    -12.39496  -0.78185  -9.30835  L
H-HC--0.017300        0    -10.92252  -1.23564  -6.70706  L
H-HC--0.017300        0    -10.4451   -0.11328  -7.96306  L
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H-HC--0.042500       0    -10.56564  -3.12116  -8.34978  L
H-HC--0.042500       0    -9.13251  -2.26304  -7.81066  L
N-N--0.415700        0    -13.56843  -2.66861  -6.85109  L
C-CT--0.025200       -1   -14.27135  -3.91319  -6.5039   L
C-C-0.597300         0    -13.52345  -4.77648  -5.50378  L
O-O--0.567900        0    -13.86862  -5.95015  -5.34713  L
H-H-0.271900         0    -13.44836  -1.95597  -6.14059  L
H-H1-0.069800        0    -14.44626  -4.5104   -7.39924  L
H-H1-0.069800        0    -15.23875  -3.65863  -6.07284  L
N-N--0.415700        0    -12.51072  -4.22052  -4.82158  L
C-CT--0.059700       -1   -11.77891  -4.9304   -3.77172  L
C-C-0.597300         0    -12.80036  -5.47559  -2.76841  L
O-O--0.567900        0    -13.72828  -4.77558  -2.36828  L
C-CT-0.130300        0    -10.71592  -4.03728  -3.07768  L
C-CT--0.043000       0    -9.39183  -3.96216  -3.85812  L
C-CT--0.320400       0    -10.29496  -4.54589  -1.68125  L
C-CT--0.066000       0    -9.47459  -3.39864  -5.26966  L
H-H-0.271900         0    -12.35396  -3.22621  -4.94736  L
H-H1-0.086900        0    -11.27616  -5.77065  -4.23239  L
H-HC-0.018700        0    -11.12379  -3.03704  -2.955    L
H-HC-0.023600        0    -8.97325  -4.95843  -3.91769  L
H-HC-0.023600        0    -8.69725  -3.33895  -3.29797  L
H-HC-0.088200        0    -9.54505  -3.87765  -1.25345  L
H-HC-0.088200        0    -9.88121  -5.55273  -1.75103  L
H-HC-0.088200        0    -11.14343  -4.54607  -1.00554  L
H-HC-0.018600        0    -8.4749   -3.3492   -5.6987   L
H-HC-0.018600        0    -9.89024  -2.39871  -5.224    L
H-HC-0.018600        0    -10.0946  -4.03325  -5.89888  L
N-N--0.415700        0    -12.6182  -6.72859  -2.34968  L
C-CT--0.025200       -1   -13.47289  -7.37073  -1.34312  L
C-C-0.597300         0    -12.91802  -7.31014   0.06306  L
O-O--0.567900        0    -13.64407  -7.10811   1.03434  L
H-H-0.271900         0    -11.87522  -7.23617  -2.81295  L
H-H1-0.069800        0    -13.60803  -8.41769  -1.60996  L
H-H1-0.069800        0    -14.4583  -6.9022   -1.33984  L
N-N--0.415700        0    -11.61009  -7.50606   0.15425  L
C-CT--0.058100       -1   -10.85576  -7.50161   1.38919  L
C-C-0.597300         0    -9.4774   -6.86084   1.12077  L
O-O--0.567900        0    -8.74331  -7.34594   0.26082  L
C-CT--0.007400       0    -10.70942  -8.94676   1.8965   L
C-CC-0.186800        0    -12.00723  -9.53344   2.40384  L
N-NB--0.543200       0    -12.60756  -9.25333   3.63466  L
C-CW--0.220700       0    -12.82411  -10.36227   1.69187  L
C-CR-0.163500        0    -13.77822  -9.90559   3.6289   L
N-NA--0.279500       0    -13.9342  -10.5843   2.47827  L
H-H-0.271900         0    -11.09008  -7.62437  -0.70349  L
H-H1-0.136000        0    -11.37379  -6.91436   2.14907  L
H-HC-0.036700        0    -9.97261  -8.97577   2.69676  L
H-HC-0.036700        0    -10.32665  -9.57403   1.08995  L
H-H4-0.186200        0    -12.63901  -10.72253   0.69013  L
H-H-0.333900         0    -14.75146  -11.12027   2.2269   L
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H-H5-0.143500        0    -14.49865  -9.87589   4.43621  L
N-N--0.415700        0    -9.12543   -5.7592    1.79629  L
C-CT--0.024900       -1   -7.8633    -5.02839   1.56403  L
C-C-0.597300         0    -6.67204   -5.66259   2.28349  L
O-O--0.567900        0    -6.71404   -5.93792   3.48224  L
C-CT-0.211700        0    -7.98658   -3.53568   1.89543  L
O-OH--0.654600       0    -6.70854   -2.91227   1.85765  L
H-H-0.271900         0    -9.738     -5.46504   2.54911  L
H-H1-0.084300        0    -7.65272   -5.07462   0.49485  L
H-H1-0.035200        0    -8.42531   -3.42046   2.87971  L
H-H1-0.035200        0    -8.64498   -3.05647   1.16853  L
H-HO-0.427500        0    -6.71884   -2.15108   2.46892  L
N-N--0.415700        0    -5.58133   -5.86142   1.54108  L
C-CT--0.051800       -1   -4.27945   -6.26494   2.06781  L
C-C-0.597300         0    -3.39348   -5.05203   2.28763  L
O-O--0.567900        0    -3.1932    -4.26408   1.36465  L
C-CT--0.110200       0    -3.60126   -7.2504    1.09172  L
C-CT-0.353100        0    -4.11431   -8.70327   1.11778  L
C-CT--0.412100       0    -5.50304   -8.87728   0.50185  L
C-CT--0.412100       0    -3.14631   -9.58521   0.32223  L
H-H-0.271900         0    -5.65949   -5.64689   0.55886  L
H-H1-0.092200        0    -4.41334   -6.76814   3.02861  L
H-HC-0.045700        0    -2.54522   -7.28338   1.35004  L
H-HC-0.045700        0    -3.66948   -6.86419   0.07741  L
H-HC--0.036100       0    -4.13299   -9.0586    2.14835  L
H-HC-0.100000        0    -5.5259    -8.46401  -0.50714  L
H-HC-0.100000        0    -6.25183   -8.37648   1.11322  L
H-HC-0.100000        0    -5.7638    -9.93382   0.46251  L
H-HC-0.100000        0    -2.14772   -9.52241   0.75389  L
H-HC-0.100000        0    -3.11407   -9.25694  -0.71732  L
H-HC-0.100000        0    -3.47944   -10.62221   0.35809  L
N-N--0.415700        0    -2.82854   -4.94395   3.4823   L
C-CT-0.021300        -1   -1.90239   -3.87861   3.83417  L
C-C-0.597300         0    -0.76298   -4.39771   4.72933  L
O-O--0.567900        0    -0.77124   -5.5582    5.14396  L
C-CT--0.123100       0    -2.73283   -2.77444   4.49601  L
S-SH--0.311900       0    -1.81265   -1.21912   4.58586  L
H-H-0.271900         0    -3.07214   -5.61544   4.20219  L
H-H1-0.112400        0    -1.4461    -3.46996   2.92919  L
H-H1-0.111200        0    -3.03946   -3.08543   5.49628  L
H-H1-0.111200        0    -3.62476   -2.59828   3.89423  L
H-HS-0.193300        0    -2.73067   -0.55833   5.30565  L
N-N--0.415700        0     0.2261    -3.56515   5.05369  L
C-CT--0.038900       -1    1.33318   -3.94038   5.94586  L
C-C-0.597300         0     1.45496   -3.05079   7.15948  L
O-O--0.567900        0     0.78255   -2.03786   7.3262   L
C-CT-0.365400        0     2.69107   -4.06482   5.22539  L
O-OH--0.676100       0     3.10292   -2.86348   4.6098   L
C-CT--0.243800       0     2.68711   -5.19537   4.19979  L
H-H-0.271900         0     0.14156   -2.60616   4.73729  L
H-H1-0.100700        0     1.12186   -4.92968   6.35149  L
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H-H1-0.004300        0     3.45393  -4.32879   5.95779  L
H-HC-0.064200        0     1.97526  -4.99142   3.40188  L
H-HC-0.064200        0     2.40568  -6.13068   4.68467  L
H-HC-0.064200        0     3.68257  -5.30039   3.77806  L
H-HO-0.410200        0     3.45897  -2.26707   5.30745  L
N-N--0.415700        0     2.30178  -3.53106   8.06073  L
C-CT--0.051800       -1    2.22015  -3.23599   9.46809  L
C-C-0.597300         0     2.30719  -1.73762   9.84878  L
O-O--0.567900        0     1.74718  -1.34884   10.86433  L
C-CT--0.110200       0     3.22743  -4.10627   10.18815  L
C-CT-0.353100        0     2.92803  -4.18717   11.68668  L
C-CT--0.412100       0     1.5884   -4.83868   12.04192  L
C-CT--0.412100       -1    4.02322  -5.0809    12.2062  L
H-H-0.271900         0     2.76735  -4.384     7.80729  L
H-H1-0.092200        0     1.21903  -3.54501   9.7699   L
H-HC-0.045700        0     4.22365  -3.69107   10.02704  L
H-HC-0.045700        0     3.18913  -5.11398   9.76931  L
H-HC--0.036100       0     3.01481  -3.21135   12.16116  L
H-HC-0.100000        0     1.47075  -5.7929    11.5298  L
H-HC-0.100000        0     0.76653  -4.17881   11.77126  L
H-HC-0.100000        0     1.52692  -4.99361   13.12008  L
H-HC-0.100000        0     3.91645  -5.17432   13.28775  L
H-HC-0.100000        0     4.99961  -4.64149   12.00431  L
H-HC-0.100000        0     3.95737  -6.07492   11.76399  L
N-N--0.516300        0     2.97681  -0.89125   9.06138  L
C-CT-0.039700        -1    3.10722   0.56197   9.3089   L
C-C-0.536600         0     1.86188   1.41413   8.96839  L
O-O--0.581900        0     1.94352   2.64433   8.92647  L
C-CT-0.056000        0     4.36891   1.07133   8.57437  L
C-CT-0.013600        0     4.36528   0.95451   7.03594  L
C-C-0.805400         0     4.97192  -0.35247   6.5109   L
O-O2--0.818800       0     4.31608  -1.42236   6.54502  L
O-O2--0.818800       0     6.15995  -0.34856   6.09512  L
H-H-0.293600         0     3.31787  -1.25506   8.17594  L
H-H1-0.110500        0     3.26914   0.71303   10.37721  L
H-HC--0.017300       0     5.24217   0.54458   8.9633   L
H-HC--0.017300       0     4.50499   2.12273   8.83045  L
H-HC--0.042500       0     4.97771   1.76906   6.64766  L
H-HC--0.042500       0     3.35526   1.08367   6.65077  L
N-N--0.415700        0     0.71293   0.76615   8.76261  L
C-CT--0.002400       -1   -0.60237   1.38283   8.55226  L
C-C-0.597300         0    -1.73704   0.74146   9.36651  L
O-O--0.567900        0    -2.91505   1.05256   9.17832  L
C-CT--0.034300       0    -0.976     1.2184    7.06841  L
C-CA-0.011800        0    -0.0469    1.77843   6.00697  L
C-CA--0.125600       0    -0.22814   3.09562   5.55159  L
C-CA--0.125600       0     0.89443   0.9469    5.36903  L
C-CA--0.170400       0     0.49266   3.5652    4.44158  L
C-CA--0.170400       0     1.64882   1.42937   4.28411  L
C-CA--0.107200       0     1.43887   2.73617   3.81361  L
H-H-0.271900         0     0.77028  -0.24199   8.70561  L
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H-H1-0.097800        0    -0.56125   2.44413   8.79691  L
H-HC-0.029500        0    -1.95231   1.67457   6.90721  L
H-HC-0.029500        0    -1.09657   0.15171   6.8849   L
H-HA-0.133000        0    -0.94854   3.73949   6.03503  L
H-HA-0.133000        0     1.02123  -0.07259   5.70015  L
H-HA-0.143000        0     0.30817   4.5685    4.08593  L
H-HA-0.143000        0     2.36916   0.78975   3.7938   L
H-HA-0.129700        0     2.00946   3.09836   2.97065  L
N-N--0.415700        0    -1.37436  -0.17056   10.25761  L
C-CT--0.003100      -1    -2.23727  -1.05055   11.02788  L
C-C-0.597300         0    -3.48021  -0.35551   11.64216  L
O-O--0.567900        0    -4.6208   -0.7042    11.35404  L
C-CT--0.003600       0    -1.3172   -1.64504   12.11482  L
C-CT--0.064500       0    -1.97443  -2.38961   13.28996  L
C-C-0.695100         0    -1.04374  -2.43035   14.50097  L
O-O--0.608600        0    -0.58861  -3.47806   14.93117  L
N-N--0.940700        0    -0.7247   -1.30637   15.11181  L
H-H-0.271900         0    -0.37768  -0.24568   10.4201  L
H-H1-0.085000        0    -2.61139  -1.84839   10.39996  L
H-HC-0.017100        0    -0.73346  -0.82195   12.53028  L
H-HC-0.017100        0    -0.61211  -2.32259   11.63544  L
H-HC-0.035200        0    -2.22011  -3.40549   12.97951  L
H-HC-0.035200        0    -2.89294  -1.90212   13.60873  L
H-H-0.425100         0    -0.08922  -1.42285   15.87444  L
H-H-0.425100         0    -0.99195  -0.37425   14.78371  L
N-N--0.516300        0    -3.26175   0.56867   12.57152  L
C-CT-0.038100       -1    -4.23518   1.43411   13.27527  L
C-C-0.536600         0    -4.80966   2.51172   12.35279  L
O-O--0.581900        0    -6.00044   2.81581   12.41861  L
C-CT--0.030300       0    -3.51272   2.06484   14.48358  L
C-C-0.799400         0    -2.04991   2.37441   14.14753  L
O-O2--0.801400       0    -1.79827   3.38297   13.45267  L
O-O2--0.801400       0    -1.2091    1.46589   14.36265  L
H-H-0.293600         0    -2.28193   0.72824   12.78158  L
H-H1-0.088000        0    -5.07144   0.83454   13.63567  L
H-HC--0.012200       0    -3.53834   1.35419   15.31172  L
H-HC--0.012200       0    -4.03007   2.97189   14.80073  L
N-N--0.415700        0    -3.9663    3.05856   11.47274  L
C-CT-0.014300       -1    -4.32013   4.07484   10.48568  L
C-C-0.597300         0    -5.57107   3.73742   9.67542  L
O-O--0.567900        0    -6.36639   4.62016   9.35399  L
C-CT--0.204100       0    -3.11811   4.3908    9.57576  L
C-C-0.713000         0    -2.12504   5.38867   10.14542  L
O-O--0.593100        0    -1.72121   6.31865   9.46873  L
N-N--0.919100        0    -1.65335   5.25198   11.36333  L
H-H-0.271900         0    -3.00668   2.75142   11.53705  L
H-H1-0.104800        0    -4.57419   4.98929   11.02521  L
H-HC-0.079700        0    -3.49929   4.82702   8.65006  L
H-HC-0.079700        0    -2.58593   3.4872    9.30835  L
H-H-0.419600         0    -1.01172   5.97715   11.61648  L
H-H-0.419600         0    -1.90865   4.52601   12.03603  L
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N-N--0.347900        0    -5.76404   2.44997   9.38414  L
C-CT--0.263700       -1   -6.91108   1.94858   8.63542  L
C-C-0.734100         0    -8.30688   2.25927   9.19377  L
O-O--0.589400        0    -9.29549   2.05189   8.49237  L
C-CT--0.000700       0    -6.73222   0.44728   8.34681  L
C-CT-0.039000        0    -7.31917  -0.44093   9.44818  L
C-CT-0.048600        0    -6.91319  -1.90222   9.2771   L
N-N2--0.529500       0    -7.58769  -2.70578   10.30286  L
C-CA-0.807600        0    -7.07616  -3.0924    11.44607  L
N-N2--0.862700       0    -5.80387  -3.19289   11.66729  L
N-N2--0.862700       0    -7.86088  -3.33338   12.44694  L
H-H-0.274700         0    -5.03009   1.81054   9.66979  L
H-H1-0.156000        0    -6.88152   2.45796   7.66995  L
H-HC-0.032700        0    -5.66977   0.22623   8.22912  L
H-HC-0.032700        0    -7.2373    0.20795   7.40949  L
H-HC-0.028500        0    -8.40809  -0.38131   9.4213   L
H-HC-0.028500        0    -6.976    -0.08744   10.42091  L
H-H1-0.068700        0    -5.8314   -1.97008   9.36739  L
H-H1-0.068700        0    -7.20012  -2.25915   8.29119  L
H-H-0.345600         0    -8.59704  -2.76083   10.25618  L
H-H-0.447800         0    -5.42861  -2.25683   11.77253  L
H-H-0.447800         0    -5.32803  -3.54221   10.82567  L
H-H-0.447800         0    -7.43037  -3.57754   13.31344  L
H-H-0.447800         0    -8.83516  -3.04989   12.35036  L
N-N--0.415700        0    -8.42325   2.72225   10.43485  L
C-CT--0.149000       -1   -9.70754   3.06112   11.02172  L
H-H-0.271900         0    -7.56818   2.85847   10.96319  L
H-H1-0.097600        0    -10.28908   3.67413   10.33209  L
H-H1-0.097600        0    -9.55154   3.61247   11.94958  L
H-H1-0.097600        0    -10.25842   2.14366   11.2388  L
C-CT--0.366200       -1   -9.91478   6.27537   8.83269  L
C-C-0.597200         0    -10.6336   5.53521   7.72936  L
O-O--0.567900        0    -11.81581   5.78136   7.53025  L
H-HC-0.112300        0    -9.09936   5.66771   9.22575  L
H-HC-0.112300        0    -10.62064   6.50334   9.62829  L
H-HC-0.112300        0    -9.51118   7.20038   8.42504  L
N-N--0.415700        0    -9.94477   4.62038   7.0435   L
C-CT--0.001400       -1   -10.47178   3.77847   5.94915  L
C-C-0.597300         0    -11.80444   3.07842   6.25335  L
O-O--0.567900        0    -12.68043   2.94064   5.39644  L
C-CT--0.015200       0    -9.33731   2.88082   5.40241  L
C-CA--0.001100       0    -9.73063   1.64962   4.60655  L
C-CA--0.190600       0    -10.33852   0.56028   5.25957  L
C-CA--0.190600       0    -9.42174   1.55849   3.23476  L
C-CA--0.234100       0    -10.68618  -0.59139   4.534    L
C-CA--0.234100       0    -9.72522   0.38731   2.51312  L
C-C-0.322600         0    -10.36786  -0.68394   3.16416  L
O-OH--0.557900       0    -10.69574  -1.80792   2.48376  L
H-H-0.271900         0    -8.97523   4.49822   7.29553  L
H-H1-0.087600        0    -10.71916   4.45971   5.13335  L
H-HC-0.029500        0    -8.70613   2.54037   6.21563  L
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H-HC-0.029500        0    -8.69513   3.50627   4.78083  L
H-HA-0.169900        0    -10.54683   0.61655   6.31867  L
H-HA-0.169900        0    -8.93445   2.38379   2.73405  L
H-HA-0.165600        0    -11.18223  -1.41272   5.02207  L
H-HA-0.165600        0    -9.48387   0.30154   1.46219  L
H-HO-0.399200        0    -11.60203  -2.04326   2.75038  L
N-N--0.516300        0    -11.97239   2.65885   7.49986  L
C-CT-0.038100        -1   -13.19999   2.0924    8.03561  L
C-C-0.536600         0    -14.40232   3.05221   8.19741  L
O-O--0.581900        0    -15.538    2.55876   8.24216  L
C-CT--0.030300       0    -12.87231   1.52074   9.43907  L
C-C-0.799400         0    -12.17417   0.1556    9.42849  L
O-O2--0.801400       0    -12.68929  -0.75734   8.74395  L
O-O2--0.801400       0    -11.18014  -0.05729   10.15197  L
H-H-0.293600         0    -11.14274   2.70823   8.08367  L
H-H1-0.088000        0    -13.5216   1.27918   7.38474  L
H-HC--0.012200       0    -13.80145   1.39382   9.99665  L
H-HC--0.012200       0    -12.27258   2.24359   9.99287  L
N-N--0.415700        0    -14.16152   4.36106   8.38692  L
C-CT--0.149000       -1   -15.10941   5.40429   8.80688  L
H-H-0.271900         0    -13.20721   4.66077   8.20275  L
H-H1-0.097600        0    -16.01481   5.34011   8.20128  L
H-H1-0.097600        0    -14.65381   6.38608   8.66655  L
H-H1-0.097600        0    -15.36761   5.26816   9.8574   L
C-CT--0.366200       -1   -19.78749  -1.13547  -1.30457  L
C-C-0.597200         0    -18.78809  -0.78341  -0.19127  L
O-O--0.567900        0    -18.39982   0.37494  -0.11176  L
H-HC-0.112300        0    -20.64396  -1.65161  -0.87796  L
H-HC-0.112300        0    -19.28846  -1.76536  -2.03956  L
H-HC-0.112300        0    -20.11358  -0.21525  -1.78764  L
N-N--0.415700        0    -18.35947  -1.72877   0.67468  L
C-CT--0.058100       -1   -17.23205  -1.51      1.63077  L
C-C-0.597300         0    -16.38663  -2.74285   1.96438  L
O-O--0.567900        0    -16.81316  -3.56736   2.77774  L
C-CT--0.007400       0    -17.66739  -0.73589   2.88603  L
C-CC-0.186800        0    -16.48052  -0.00563   3.4714   L
N-NB--0.543200       0    -15.43645  -0.61967   4.15445  L
C-CW--0.220700       0    -16.15351   1.30459   3.26605  L
C-CR-0.163500        0    -14.47743   0.31134   4.3036   L
N-NA--0.279500       0    -14.90149   1.49034   3.82421  L
H-H-0.271900         0    -18.7155  -2.66495   0.56641  L
H-H1-0.136000        0    -16.57585  -0.80586   1.12463  L
H-HC-0.036700        0    -18.09107  -1.41554   3.62575  L
H-HC-0.036700        0    -18.42509   0.00182   2.6201   L
H-H4-0.186200        0    -16.72924   2.02373   2.69746  L
H-H-0.333900         0    -14.33182   2.33483   3.85157  L
H-H5-0.143500        0    -13.50618   0.14688   4.75661  L
N-N--0.254800        0    -15.18266  -2.87015   1.37599  L
C-CT--0.026600       -1   -14.22911  -3.88769   1.78373  L
C-C-0.589600         0    -13.53557  -3.56016   3.09639  L
O-O--0.574800        0    -13.13805  -2.41991   3.33612  L
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C-CT--0.007000       0    -13.18451  -3.93069   0.67713  L
C-CT-0.018900        0    -13.21    -2.53727   0.0515   L
C-CT-0.019200        0    -14.65203  -2.08661   0.259    L
H-H1-0.064100        0    -14.72062  -4.85835   1.86105  L
H-HC-0.025300        0    -13.51347  -4.66551  -0.04164  L
H-HC-0.025300        0    -12.19242  -4.1913    1.04912  L
H-HC-0.021300        0    -12.94203  -2.55724  -1.00524  L
H-HC-0.021300        0    -12.54259  -1.87033   0.59516  L
H-H1-0.039100        0    -14.65573  -1.01744   0.47284  L
H-H1-0.039100        0    -15.23271  -2.29581  -0.64091  L
N-N--0.347900        0    -13.26816  -4.57975   3.91428  L
C-CT--0.263700      -1    -12.50311  -4.40282   5.15533  L
C-C-0.734100         0    -10.99371  -4.74588   4.97975  L
O-O--0.589400        0    -10.67037  -5.5975    4.15753  L
C-CT--0.000700       0    -13.22625  -5.05412   6.34699  L
C-CT-0.039000        0    -14.54381  -4.30663   6.67604  L
C-CT-0.048600        0    -14.32902  -2.9242    7.33129  L
N-N2--0.529500       0    -15.24216  -1.87872   6.81225  L
C-CA-0.807600        0    -15.65256  -0.78044   7.43206  L
N-N2--0.862700       0    -15.36805  -0.51387   8.66639  L
N-N2--0.862700       0    -16.3244   0.14057   6.81073  L
H-H-0.274700         0    -13.53742  -5.50611   3.60812  L
H-H1-0.156000        0    -12.47771  -3.33784   5.37727  L
H-HC-0.032700        0    -12.5778  -5.03959   7.22499  L
H-HC-0.032700        0    -13.45107  -6.09321   6.10322  L
H-HC-0.028500        0    -15.12822  -4.91869   7.36364  L
H-HC-0.028500        0    -15.13291  -4.19474   5.76459  L
H-H1-0.068700        0    -13.30746  -2.59396   7.14892  L
H-H1-0.068700        0    -14.4463  -3.03027   8.41126  L
H-H-0.345600         0    -15.43292  -1.8863    5.8153   L
H-H-0.447800         0    -15.59507   0.40946   8.99163  L
H-H-0.447800         0    -14.47808  -0.93211   8.93937  L
H-H-0.447800         0    -16.40014   1.05413   7.24205  L
H-H-0.447800         0    -16.36008   0.05515   5.80172  L
N-N--0.415700        0    -10.06678  -4.0358    5.65456  L
C-CT--0.003100      -1    -8.58072  -4.14107   5.53506  L
C-C-0.597300         0    -7.98163  -4.97877   6.67178  L
O-O--0.567900        0    -8.43649  -4.90187   7.81489  L
C-CT--0.003600       0    -7.95045  -2.74212   5.49715  L
C-CT--0.064500       0    -6.41669  -2.81789   5.40207  L
C-C-0.695100         0    -5.82817  -1.49173   4.9741   L
O-O--0.608600        0    -6.06986  -1.05749   3.86066  L
N-N--0.940700        0    -5.03411  -0.83617   5.78649  L
H-H-0.271900         0    -10.41035  -3.35202   6.31923  L
H-H1-0.085000        0    -8.35738  -4.64832   4.6026   L
H-HC-0.017100        0    -8.23043  -2.18152   6.38737  L
H-HC-0.017100        0    -8.34172  -2.20426   4.63572  L
H-HC-0.035200        0    -6.12914  -3.55786   4.65604  L
H-HC-0.035200        0    -6.00338  -3.11475   6.3634   L
H-H-0.425100         0    -4.75907   0.10742   5.53921  L
H-H-0.425100         0    -4.70924  -1.3045    6.64327  L
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N-N--0.415700        0    -6.92724  -5.73416   6.35858  L
C-CT--0.001400       -1   -6.18174  -6.56116   7.30241  L
C-C-0.597300         0    -4.67836  -6.50687   7.00959  L
O-O--0.567900        0    -4.23963  -6.68029   5.86671  L
C-CT--0.015200       0    -6.66859  -8.02204   7.24033  L
C-CA--0.001100       0    -8.16655  -8.20526   7.07739  L
C-CA--0.190600       0    -9.01131  -8.37099   8.19421  L
C-CA--0.190600       0    -8.71509  -8.15968   5.78275  L
C-CA--0.234100       0    -10.40437  -8.50608   8.0111   L
C-CA--0.234100       0    -10.10122  -8.26935   5.60559  L
C-C-0.322600         0    -10.94984  -8.45915   6.71022  L
O-OH--0.557900       0    -12.28359  -8.60164   6.499    L
H-H-0.271900         0    -6.64301  -5.7723    5.38418  L
H-H1-0.087600        0    -6.35207  -6.18302   8.31163  L
H-HC-0.029500        0    -6.33782  -8.53822   8.14223  L
H-HC-0.029500        0    -6.18592  -8.51523   6.39482  L
H-HA-0.169900        0    -8.59216  -8.37927   9.18983  L
H-HA-0.169900        0    -8.07527  -7.9963    4.92498  L
H-HA-0.165600        0    -11.06792  -8.63363   8.85162  L
H-HA-0.165600        0    -10.52393  -8.17406   4.62352  L
H-HO-0.399200        0    -12.42377  -8.70384   5.5453   L
N-N--0.516300        0    -3.87539  -6.28211   8.04705  L
C-CT-0.039700        -1   -2.42499  -6.20232   7.91844  L
C-C-0.536600         0    -1.73178  -7.57354   7.99406  L
O-O--0.581900        0    -1.95143  -8.35934   8.91594  L
C-CT-0.056000        0    -1.81211  -5.21188   8.91664  L
C-CT-0.013600        0    -2.07871  -3.75749   8.49813  L
C-C-0.805400         0    -3.55843  -3.34684   8.59723  L
O-O2--0.818800       0    -4.25525  -3.83733   9.51948  L
O-O2--0.818800       0    -4.00609  -2.53535   7.75705  L
H-H-0.293600         0    -4.28629  -5.97442   8.92069  L
H-H1-0.110500        0    -2.21876  -5.8045    6.93115  L
H-HC--0.017300       0    -0.72987  -5.35469   8.92198  L
H-HC--0.017300       0    -2.18121  -5.40308   9.92528  L
H-HC--0.042500       0    -1.72598  -3.62071   7.4739   L
H-HC--0.042500       0    -1.47039  -3.11175   9.13127  L
N-N--0.415700        0    -0.84642  -7.853     7.03108  L
C-CT--0.002400       -1   -0.08998  -9.10751   6.92033  L
C-C-0.597300         0     1.41355  -8.87706   7.0949   L
O-O--0.567900        0     1.93294  -7.75699   7.12479  L
C-CT--0.034300       0    -0.43817  -9.78703   5.57657  L
C-CA-0.011800        0     0.12054  -9.09781   4.33924  L
C-CA--0.125600       0    -0.60384  -8.07848   3.69584  L
C-CA--0.125600       0     1.39164  -9.44924   3.85003  L
C-CA--0.170400       0    -0.02831  -7.36838   2.62518  L
C-CA--0.170400       0     1.97068  -8.7391    2.78269  L
C-CA--0.107200       0     1.26055  -7.69209   2.17308  L
H-H-0.271900         0    -0.71408  -7.14658   6.31196  L
H-H1-0.097800        0    -0.41224  -9.77549   7.71991  L
H-HC-0.029500        0    -1.52429  -9.84859   5.48596  L
H-HC-0.029500        0    -0.06675  -10.81186   5.59808  L
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H-HA-0.133000        0    -1.5845   -7.79994   4.0581   L
H-HA-0.133000        0     1.92957  -10.25946   4.31073  L
H-HA-0.143000        0    -0.55946  -6.54312   2.17226  L
H-HA-0.143000        0     2.96062  -8.99009   2.435    L
H-HA-0.129700        0     1.69986  -7.12263   1.36709  L
N-N--0.415700        0     2.14336  -9.98158   7.23308  L
C-CT--0.024900       -1    3.58735  -9.93709   7.4219   L
C-C-0.597300         0     4.33891  -9.44465   6.16814  L
O-O--0.567900        0     4.21205  -10.00656   5.08241  L
C-CT-0.211700        0     4.12951  -11.31456   7.84428  L
O-OH--0.654600       0     3.88161  -12.33823   6.8864   L
H-H-0.271900         0     1.66017  -10.86157   7.167    L
H-H1-0.084300        0     3.79645  -9.24136   8.2355   L
H-H1-0.035200        0     3.67632  -11.59873   8.79558  L
H-H1-0.035200        0     5.20692  -11.23175   7.99662  L
H-HO-0.427500        0     3.10995  -12.83721   7.18353  L
N-N--0.347900        0     5.1958   -8.43036   6.31445  L
C-CT--0.263700       -1    6.08692  -7.90554   5.25535  L
C-C-0.734100         0     7.16603  -8.90388   4.80007  L
O-O--0.589400        0     7.22563  -10.04305   5.26865  L
C-CT--0.000700       0     6.65682  -6.56565   5.77093  L
C-CT-0.039000        0     7.77496  -6.69527   6.82124  L
C-CT-0.048600        0     8.11627  -5.35898   7.4968   L
N-N2--0.529500       0     8.4213   -4.27924   6.53319  L
C-CA-0.807600        0     7.65352  -3.2509    6.21471  L
N-N2--0.862700       0     6.44422  -3.14636   6.67251  L
N-N2--0.862700       0     8.07094  -2.2902    5.44831  L
H-H-0.274700         0     5.18883  -7.9816    7.217    L
H-H1-0.156000        0     5.46709  -7.69237   4.3815   L
H-HC-0.032700        0     5.83595  -5.9804    6.1899   L
H-HC-0.032700        0     7.05104  -5.99784   4.93665  L
H-HC-0.028500        0     8.67422  -7.08048   6.34373  L
H-HC-0.028500        0     7.47034  -7.4       7.59552  L
H-H1-0.068700        0     8.9886   -5.5128    8.13449  L
H-H1-0.068700        0     7.28983  -5.07016   8.14762  L
H-H-0.345600         0     9.35143  -4.2754    6.12205  L
H-H-0.447800         0     5.89212  -2.31165   6.43322  L
H-H-0.447800         0     6.04932  -3.81332   7.293    L
H-H-0.447800         0     7.40492  -1.52147   5.3358   L
H-H-0.447800         0     8.96881  -2.28575   4.99209  L
N-N--0.415700        0     8.03851  -8.46098   3.90132  L
C-CT--0.051800       -1    9.37771  -9.00028   3.64868  L
C-C-0.597300         0     10.30038  -7.79498   3.82816  L
O-O--0.567900        0     10.34587  -6.8948    2.99446  L
C-CT--0.110200       0     9.40334  -9.63696   2.24371  L
C-CT-0.353100        0     10.73441  -10.29417   1.82365  L
C-CT--0.412100       0     10.45816  -11.37212   0.77249  L
C-CT--0.412100       0     11.72329  -9.31515   1.19278  L
H-H-0.271900         0     7.85773  -7.54276   3.50094  L
H-H1-0.092200        0     9.63142  -9.76192   4.38846  L
H-HC-0.045700        0     9.10856  -8.90201   1.49331  L
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H-HC-0.045700        0     8.64383  -10.41312   2.2477   L
H-HC--0.036100       0     11.1947  -10.76722   2.69129  L
H-HC-0.100000        0     11.39418  -11.8465   0.47584  L
H-HC-0.100000        0     9.99437  -10.92395  -0.10839  L
H-HC-0.100000        0     9.80069  -12.13767   1.1816   L
H-HC-0.100000        0     12.61699  -9.85061   0.87458  L
H-HC-0.100000        0     12.01833  -8.55067   1.90349  L
H-HC-0.100000        0     11.26961  -8.83503   0.32694  L
N-N--0.415700        0     10.98204  -7.73398   4.96581  L
C-CT-0.014300        -1    12.26554  -7.0585    4.99781  L
C-C-0.597300         0     13.29778  -8.12411   4.54172  L
O-O--0.567900        0     13.2888  -9.21331   5.11603  L
C-CT--0.204100       0     12.61614  -6.57938   6.41768  L
C-C-0.713000         0     11.84827  -5.3599    6.88472  L
O-O--0.593100        0     11.15399  -4.67839   6.14766  L
N-N--0.919100        0     11.94926  -5.03603   8.15173  L
H-H-0.271900         0     10.9027  -8.5254    5.58627  L
H-H1-0.104800        0     12.29247  -6.21571   4.30507  L
H-HC-0.079700        0     13.67525  -6.31748   6.43576  L
H-HC-0.079700        0     12.46297  -7.39533   7.12421  L
H-H-0.419600         0     11.48887  -4.19115   8.43393  L
H-H-0.419600         0     12.56301  -5.55521   8.75801  L
N-N--0.415700        0     14.12764  -7.87837   3.51676  L
C-CT--0.051800       -1    15.23125  -8.78812   3.15145  L
C-C-0.597300         0     16.44417  -8.5659    4.09347  L
O-O--0.567900        0     16.71266  -7.42847   4.47635  L
C-CT--0.110200       0     15.60115  -8.6407    1.64128  L
C-CT-0.353100        0     16.61661  -9.67192   1.065    L
C-CT--0.412100       0     16.12029  -11.11065   1.25047  L
C-CT--0.412100       -1    16.89761  -9.51014  -0.44926  L
H-H-0.271900         0     14.0977  -6.98129   3.05502  L
H-H1-0.092200        0     14.88038  -9.8068    3.31208  L
H-HC-0.045700        0     16.00763  -7.64293   1.48098  L
H-HC-0.045700        0     14.68597  -8.7115    1.05526  L
H-HC--0.036100       0     17.5611  -9.56411   1.59361  L
H-HC-0.100000        0     15.14212  -11.23263   0.78577  L
H-HC-0.100000        0     16.05769  -11.35928   2.30733  L
H-HC-0.100000        0     16.82581  -11.80235   0.78931  L
H-HC-0.100000        0     15.99976  -9.72714  -1.02398  L
H-HC-0.100000        0     17.69597  -10.18897  -0.74914  L
H-HC-0.100000        0     17.2238  -8.48752  -0.64296  L
N-N--0.516300        0     17.1714  -9.62487   4.48197  L
C-CT-0.039700        -1    18.42685  -9.50122   5.26178  L
C-C-0.536600         0     19.50794  -8.6924    4.4873   L
O-O--0.581900        0     19.43801  -8.56191   3.26205  L
C-CT-0.056000        0     18.96093  -10.87597   5.7083   L
C-CT-0.013600        0     18.66446  -11.15058   7.19262  L
C-C-0.805400         0     19.2237  -10.07168   8.14187  L
O-O2--0.818800       0     18.69896  -9.97845   9.27103  L
O-O2--0.818800       0     20.11853  -9.30495   7.70843  L
H-H-0.293600         0     16.91757  -10.53736   4.14715  L
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H-H1-0.110500        0     18.19548  -8.90268   6.14372  L
H-HC--0.017300       0     20.04077  -10.92018   5.55861  L
H-HC--0.017300       0     18.51563  -11.66473   5.09914  L
H-HC--0.042500       0     19.09241  -12.12028   7.45649  L
H-HC--0.042500       0     17.58071  -11.2189   7.31617  L
N-N--0.415700        0     20.4759  -8.0775    5.18519  L
C-CT--0.025200       -1    21.4836  -7.14308   4.62127  L
C-C-0.597300         0     20.86947  -5.87346   3.96537  L
O-O--0.567900        0     21.61726  -5.10694   3.36219  L
H-H-0.271900         0     20.49937  -8.30075   6.1847   L
H-H1-0.069800        0     22.06682  -7.66479   3.86265  L
H-H1-0.069800        0     22.15836  -6.8244    5.4149   L
N-N--0.415700        0     19.54497  -5.61885   4.05023  L
C-CT--0.038900       0     18.81108  -4.71194   3.1266   L
C-C-0.597300         0     17.84712  -3.71156   3.80746  L
O-O--0.567900        0     17.02586  -4.06107   4.6526   L
C-CT-0.365400        0     18.01307  -5.53062   2.08932  L
O-OH--0.676100       0     18.78396  -6.5539    1.5005   L
C-CT--0.243800       0     17.54294  -4.68094   0.90695  L
H-H-0.271900         0     18.98744  -6.27677   4.57986  L
H-H1-0.100700        0     19.54714  -4.13391   2.56929  L
H-H1-0.004300        0     17.14125  -5.97044   2.5671   L
H-HC-0.064200        0     16.88449  -3.88355   1.24187  L
H-HC-0.064200        0     16.99454  -5.31318   0.20842  L
H-HC-0.064200        0     18.40425  -4.25246   0.39382  L
H-HO-0.410200        0     19.01486  -7.21301   2.18254  L
N-N--0.415700        0     17.88835  -2.43859   3.387    L
C-CT--0.087500       -1    16.98062  -1.3346    3.79528  L
C-C-0.597300         0     15.61636  -1.46812   3.08155  L
O-O--0.567900        0     15.56923  -1.48231   1.85491  L
C-CT-0.298500        0     17.57717   0.03701   3.39147  L
C-CT--0.319200       -1    16.7095   1.23883   3.86348  L
C-CT--0.319200       -1    19.02301   0.13251   3.91064  L
H-H-0.271900         0     18.56881  -2.23358   2.67079  L
H-H1-0.096900        0     16.83807  -1.3645    4.87492  L
H-HC--0.029700       0     17.63502   0.08884   2.30383  L
H-HC-0.079100        0     16.59474   1.21456   4.94639  L
H-HC-0.079100        0     15.73244   1.21801   3.38146  L
H-HC-0.079100        0     17.20577   2.16823   3.58133  L
H-HC-0.079100        0     19.04914  -0.04401   4.98619  L
H-HC-0.079100        0     19.41329   1.1304    3.70815  L
H-HC-0.079100        0     19.67232  -0.58281   3.40653  L
N-N--0.415700        0     14.49437  -1.57275   3.8129   L
C-CT--0.023700       -1    13.19123  -2.00671   3.24254  L
C-C-0.597300         0     11.92266  -1.36563   3.88383  L
O-O--0.567900        0     10.81483  -1.91324   3.82397  L
C-CT-0.034200        0     13.08293  -3.53851   3.46936  L
C-CT-0.001800        0     14.16946  -4.44969   2.87497  L
S-S--0.273700        0     13.69705  -5.3384    1.36762  L
C-CT--0.053600       0     13.80017  -3.98577   0.17123  L
H-H-0.271900         0     14.63278  -1.64478   4.80855  L
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 H-H1-0.088000        0     13.1565  -1.80306   2.1716   L
 H-HC-0.024100        0     12.12357  -3.89782   3.09435  L
 H-HC-0.024100        0     13.08556  -3.7045    4.54708  L
 H-H1-0.044000        0     14.41787  -5.19482   3.62997  L
 H-H1-0.044000        0     15.08363  -3.89847   2.6834   L
 H-H1-0.068400        0     14.79749  -3.54632   0.18991  L
 H-H1-0.068400        0     13.06567  -3.2192    0.41322  L
 H-H1-0.068400        0     13.5989  -4.37843  -0.82272  L
 N-N--0.415700        0     12.05658  -0.18974   4.50009  L
 C-CT--0.024900       -1    10.94437   0.72438   4.83586  L
 C-C-0.597300         0     11.02974   1.84803   3.80793  L
 O-O--0.567900        0     12.12373   2.37256   3.60085  L
 C-CT-0.211700        0     11.08795   1.19531   6.27921  L
 O-OH--0.654600       0     10.17519   2.21657   6.63914  L
 H-H-0.271900         0     12.97122   0.23154   4.41875  L
 H-H1-0.084300        0     9.98399   0.2193    4.72713  L
 H-H1-0.035200        0     12.10083   1.56164   6.40434  L
 H-H1-0.035200        0     10.94363   0.34047   6.94156  L
 H-HO-0.427500        0     9.28598   1.97037   6.2823   L
 N-N--0.347900        0     9.94346   2.14483   3.08164  L
 C-CT--0.240000       -1    9.9954    3.04517   1.91357  L
 C-C-0.734100         0     10.54841   4.43096   2.33206  L
 O-O--0.589400        0     11.5928   4.80065   1.80077  L
 C-CT--0.009400       0     8.63933   3.06513   1.18483  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.65698   3.68686  -0.22902  H
 C-CT--0.047900       0     7.43816   3.1889   -1.02107  H
 C-CT--0.014300       0     7.19386   3.93424  -2.32668  H
 N-N3--0.385400       0     5.8438    3.57327  -2.91501  H
 H-H-0.274700         0     9.0701    1.68907   3.32104  L
 H-H1-0.142600        0     10.72789   2.63675   1.21538  L
 H-HC-0.036200        0     7.92071   3.6007    1.79681  L
 H-HC-0.036200        0     8.29711   2.03198   1.09562  L
 H-HC-0.010300        0     9.58714   3.40775  -0.73209  H
 H-HC-0.010300        0     8.63336   4.77558  -0.1188   H
 H-HC-0.062100        0     6.53225   3.29915  -0.42605  H
 H-HC-0.062100        0     7.54032   2.12221  -1.24169  H
 H-HP-0.113500        0     7.92649   3.73523  -3.11402  H
 H-HP-0.113500        0     7.16733   5.01149  -2.16722  H
 H-H-0.340000         0     5.91687   2.84994  -3.64449  H
 H-H-0.340000         0     5.43879   4.35555  -3.46998  H
 H-H-0.340000         0     5.12878   3.2447   -2.2105   H
 N-N--0.347900        0     10.0172   5.09593   3.38735  L
 C-CT--0.263700       -1    10.65233   6.23226   4.14614  L
 C-C-0.734100         0     11.79346   5.7949    5.04092  L
 O-O--0.589400        0     11.77821   6.04541   6.24964  L
 C-CT--0.000700       0     9.57656   7.10146   4.82441  L
 C-CT-0.039000        0     8.74278   7.82183   3.74732  L
 C-CT-0.048600        0     7.72942   8.82553   4.30126  L
 N-N2--0.529500       0     6.73951   8.22007   5.21368  L
 C-CA-0.807600        0     5.48705   8.60493   5.37738  L
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N-N2--0.862700       0     4.93932   9.51943   4.63615  L
N-N2--0.862700       0     4.77662   8.06372   6.3149   L
H-H-0.274700         0     9.11183   4.76011   3.70083  L
H-H1-0.156000        0     11.13885   6.87826   3.40835  L
H-HC-0.032700        0     10.05947   7.85856   5.44464  L
H-HC-0.032700        0     8.93891   6.48057   5.45421  L
H-HC-0.028500        0     8.21551   7.09497   3.13267  L
H-HC-0.028500        0     9.41868   8.37201   3.09109  L
H-H1-0.068700        0     7.21927   9.26173   3.44172  L
H-H1-0.068700        0     8.26037   9.62332   4.82323  L
H-H-0.345600         0     7.00409   7.44087   5.79925  L
H-H-0.447800         0     3.95201   9.77172   4.72662  L
H-H-0.447800         0     5.43389   9.85635   3.8319   L
H-H-0.447800         0     3.83708   8.43173   6.47727  L
H-H-0.447800         0     5.13825   7.30905   6.86939  L
N-N--0.347900        0     12.74718   5.12733   4.3762   L
C-CT--0.240000       -1    14.14142   4.76845   4.69624  L
C-C-0.734100         0     14.99519   4.49497   3.42617  L
O-O--0.589400        0     16.20747   4.65069   3.49554  L
C-CT--0.009400       0     14.32356   3.60532   5.71346  L
C-CT-0.018700        0     13.4906   3.90011   6.95645  L
C-CT--0.047900       0     13.55245   3.07218   8.24183  L
C-CT--0.014300       0     12.5434   3.65254   9.26853  L
N-N3--0.385400       0     11.22904   4.06332   8.67912  L
H-H-0.274700         0     12.49057   5.06209   3.39772  L
H-H1-0.142600        0     14.60081   5.65304   5.14142  L
H-HC-0.036200        0     15.37613   3.53961   5.994    L
H-HC-0.036200        0     14.01948   2.65597   5.27461  L
H-HC-0.010300        0     12.47639   3.78802   6.59263  L
H-HC-0.010300        0     13.69921   4.92954   7.2511   L
H-HC-0.062100        0     14.55995   3.12117   8.6586   L
H-HC-0.062100        0     13.31949   2.02906   8.03856  L
H-HP-0.113500        0     13.0063   4.53002   9.7305   L
H-HP-0.113500        0     12.38712   2.91118   10.05736  L
H-H-0.340000         0     11.36678   4.81821   8.00588  L
H-H-0.340000         0     10.57585   4.38389   9.38022  L
H-H-0.340000         0     10.80056   3.30553   8.14751  L
N-N--0.415700        0     14.40121   4.0698    2.29859  L
C-CT--0.051800       -1    15.05953   3.65953   1.02905  L
C-C-0.597300         0     15.28216   4.76653   0.03475  L
O-O--0.567900        0     16.26183   4.74632  -0.70827  L
C-CT--0.110200       0     14.2055   2.51373   0.44368  L
C-CT-0.353100        0     14.74739   1.84967  -0.83746  L
C-CT--0.412100       0     16.12844   1.22423  -0.63597  L
C-CT--0.412100       0     13.78615   0.73974  -1.2716   L
H-H-0.271900         0     13.39886   3.94221   2.34594  L
H-H1-0.092200        0     16.04482   3.26187   1.27708  L
H-HC-0.045700        0     13.20995   2.90523   0.22769  L
H-HC-0.045700        0     14.09887   1.74139   1.20754  L
H-HC--0.036100       0     14.80071   2.58676  -1.63793  L
H-HC-0.100000        0     16.10421   0.51215   0.18807  L
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H-HC-0.100000        0     16.86275   2.00147  -0.42659  L
H-HC-0.100000        0     16.43443   0.70892  -1.54605  L
H-HC-0.100000        0     14.13754   0.29897  -2.20438  L
H-HC-0.100000        0     12.79205   1.15504  -1.43487  L
H-HC-0.100000        0     13.73615  -0.03531  -0.5057   L
N-N--0.415700        0     14.37378   5.72722   0.02182  L
C-CT-0.014300       -1     14.58145   6.94132  -0.72179  L
C-C-0.597300         0     15.65853   7.86324  -0.07726  L
O-O--0.567900        0     15.3598    8.94175   0.42902  L
C-CT--0.204100       0     13.21948   7.62624  -1.00694  L
C-C-0.713000         0     12.2246    7.72509   0.14738  L
O-O--0.593100        0     12.5297    7.5716    1.32226  L
N-N--0.919100        0     10.96607   7.9388   -0.16771  L
H-H-0.271900         0     13.60886   5.70067   0.68564  L
H-H1-0.104800        0     14.98757   6.67481  -1.6993   L
H-HC-0.079700        0     12.72884   7.06651  -1.80276  L
H-HC-0.079700        0     13.3996    8.63385  -1.38009  L
H-H-0.419600         0     10.3163    7.98194   0.59137  L
H-H-0.419600         0     10.64635   8.04486  -1.12969  L
N-N--0.415700        0     16.93299   7.43912  -0.14476  L
C-CT--0.149000      -1     18.12846   8.12333   0.36461  L
H-H-0.271900         0     17.04599   6.51297  -0.54437  L
H-H1-0.097600        0     18.1231    8.10196   1.45571  L
H-H1-0.097600        0     18.12461   9.16373   0.03388  L
H-H1-0.097600        0     19.02839   7.62903  -0.00318  L
C-CT--0.055800       0     0.85629   14.82365   4.09715  L
C-CT-0.000000        0     1.33687   13.87297   3.00282  L
O-OS--0.354800       0     2.74178   13.99407   2.8466   L
C-CT--0.202200       0     1.07846   12.41649   3.38344  L
O-OS--0.524600       0     0.69207   11.71545   2.20024  L
C-CT--0.067000       0     2.43974   11.95057   3.87558  L
O-OH--0.613900       0     2.50452   10.55321   3.76368  L
C-CT--0.006600       0     3.27373   12.68225   2.83904  L
N-N*--0.048400       0     4.72555   12.66236   3.13299  L
C-C-0.753800         0     5.54363   11.79021   2.40882  L
O-O--0.625200        0     5.09069   11.0449    1.54226  L
N-NC--0.758400       0     6.8702    11.71676   2.68483  L
C-CA-0.818500        0     7.36309   12.50204   3.61347  L
N-N2--0.953000       0     8.65022   12.40485   3.78192  L
C-CM--0.521500       0     6.58594   13.39255   4.39799  L
C-CM--0.005300       0     5.25645   13.44359   4.12939  L
H-H1-0.067900        0    -0.22887   14.7562    4.17603  L
H-H1-0.067900        0     1.30329   14.53775   5.04915  L
H-H1-0.117400        0     0.80948   14.10004   2.07329  L
H-H1-0.061500        0     0.30481   12.35598   4.14853  L
H-H1-0.097200        0     2.63724   12.30611   4.88949  L
H-HO-0.418600        0     1.74418   10.34448   3.19283  L
H-H2-0.202900        0     3.06577   12.21017   1.87429  L
H-H-0.423400         0     9.09887   11.83415   3.09018  L
H-H-0.423400         0     9.12122   13.03439   4.39963  L
H-HA-0.192800        0     7.00298   14.01821   5.16886  L
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 H-H4-0.195800        0     4.59566   14.10223   4.68281  L
 P-P-1.166200         0    -0.3537    10.48899   2.19788  L
 O-O2--0.776000       0    -1.44188   10.76911   1.24349  L
 O-O2--0.776000       0    -0.6612    10.12215   3.59832  L
 O-OS--0.498900       0     0.53561   9.27319   1.63893  L
 C-CT-0.055800        0     1.2019    9.30823   0.38933  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     1.94557   7.9736    0.14778  H
 O-OS--0.354800       0     2.82999   7.74105   1.24109  H
 C-CT-0.202200        0     1.04638   6.73485  -0.01659  H
 O-OH--0.654100       0     1.03598   6.22926  -1.33151  H
 C-CT-0.067000        0     1.65275   5.63721   0.94524  H
 O-OH--0.613900       0     2.30834   4.52963   0.38421  H
 C-CT-0.039400        0     2.73087   6.41699   1.72995  H
 N-N*--0.025100       0     2.50997   6.47014   3.1656   H
 C-CK-0.200600        0     1.5628    7.1786    3.89122  H
 N-NB--0.607300       0     1.54835   6.87962   5.1636   H
 C-CB-0.051500        0     2.50826   5.90235   5.29652  H
 C-CA-0.700900        0     2.91043   5.09685   6.38062  H
 N-N2--0.901900       0     2.39545   5.24074   7.63209  H
 N-NC--0.761500       0     3.91373   4.21975   6.19505  H
 C-CQ-0.587500        0     4.34474   4.0209    4.95087  H
 N-NC--0.699700       0     4.04544   4.70635   3.85706  H
 C-CB-0.305300        0     3.11336   5.63662   4.07274  H
 H-H1-0.067900        0     1.91737   10.13055   0.39273  L
 H-H1-0.067900        0     0.48073   9.47407  -0.41307  L
 H-H1-0.117400        0     2.52165   8.06561  -0.78719  H
 H-H1-0.061500        0     0.02254   6.96382   0.30932  H
 H-HO-0.437600        0     0.73699   6.90188  -1.98838  H
 H-H1-0.097200        0     0.85792   5.34191   1.63869  H
 H-HO-0.418600        0     5.31838   4.46157   0.92644  H
 H-H2-0.200700        0     3.68106   5.91599   1.57114  H
 H-H5-0.155300        0     0.91636   7.90738   3.42199  H
 H-H-0.411500         0     2.35725   4.36899   8.17075  H
 H-H-0.411500         0     1.49943   5.72115   7.65698  H
 H-H5-0.047300        0     5.08424   3.23976   4.81602  H
 N-N3-0.149300        0    -0.62224   4.24014  -0.23505  H
 C-CT-0.053600        0     0.17369   3.20708   0.47119  H
 C-CT-0.065100        0    -0.50384   1.8359    0.28689  H
 C-CT--0.090300       0    -0.49159   0.92506   1.52482  H
 C-C-0.735400         0    -1.51789  -0.19821   1.40254  H
 O-O--0.613300        0    -1.22975  -1.37357   1.27358  H
 N-N--1.003100        0    -2.83083   0.23423   1.33755  H
 C-C-0.612300         0     1.58282   3.30113  -0.1685   H
 O-O--0.571300        0     1.63358   3.18649  -1.41012  H
 O-OS--0.421200       0     2.40171   2.18107   0.56392  H
 P-P-1.166200         0     3.81926   1.62817   0.16305  H
 O-O2--0.776000       0     4.70527   1.58316   1.46509  H
 O-O2--0.776000       0     4.53313   2.27652  -0.99492  H
 O-OS--0.498900       0     3.73927   0.05226  -0.08971  H
 C-CT-0.055800        0     3.04841  -0.40636  -1.25827  H
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 C-CT-0.106500        0     2.50624  -1.83371  -1.03044  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.50495  -2.77515  -0.62881  L
 C-CT-0.039400        0     3.37493  -3.02245   0.77376  L
 N-N*--0.025100       0     4.70518  -2.96522   1.43141  L
 C-CB-0.305300        0     5.46692  -4.06929   1.72556  L
 N-NC--0.699700       0     5.11531  -5.37355   1.54351  L
 C-CQ-0.587500        0     6.06792  -6.20423   1.93131  L
 N-NC--0.761500       0     7.25983  -5.915     2.43615  L
 C-CA-0.700900        0     7.57843  -4.62492   2.55627  L
 N-N2--0.901900       0     8.81333  -4.43869   2.9874   L
 C-CB-0.051500        0     6.6574   -3.60347   2.21693  L
 N-NB--0.607300       0     6.67035  -2.20308   2.25432  L
 C-CK-0.200600        0     5.47313  -1.88515   1.81412  L
 C-CT-0.067000        0     2.30437  -2.08125   1.33174  L
 O-OH--0.613900       0     1.57113  -2.65264   2.40097  L
 C-CT-0.202200        0     1.45771  -1.8846    0.06951  L
 O-OH--0.654100       0     0.5825   -2.99182  -0.13229  L
 H-H-0.199600         0    -1.43897   3.51612  -1.56826  H
 H-H-0.199600         0    -0.02835   4.84131  -0.80092  H
 H-H-0.199600         0    -1.16654   4.81067   0.40826  H
 H-HP-0.101500        0     0.23325   3.43885   1.54392  H
 H-HC-0.005000        0    -0.07025   1.32577  -0.58043  H
 H-HC-0.005000        0    -1.54712   2.0346    0.02468  H
 H-HC-0.033100        0    -0.74869   1.51916   2.41391  H
 H-HC-0.033100        0     0.48841   0.48302   1.70027  H
 H-H-0.442900         0    -3.51676  -0.46734   1.57789  H
 H-H-0.442900         0    -3.01217   1.11708   1.82867  H
 H-H1-0.067900        0     3.73495  -0.41798  -2.1117   H
 H-H1-0.067900        0     2.21113   0.25202  -1.48789  H
 H-H1-0.117400        0     2.03818  -2.14966  -1.96225  L
 H-H2-0.200700        0     2.97583  -4.02951   0.90455  L
 H-H5-0.047300        0     5.84184  -7.25492   1.82257  L
 H-H-0.411500         0     9.19103  -3.50585   3.04424  L
 H-H-0.411500         0     9.39468  -5.26942   3.04136  L
 H-H5-0.155300        0     5.13165  -0.86136   1.71883  L
 H-H1-0.097200        0     2.73299  -1.13009   1.64459  L
 H-HO-0.418600        0     2.13543  -2.6748    3.19964  L
 H-H1-0.061500        0     0.90078  -0.95159   0.0932   L
 H-HO-0.437600        0    -0.16088  -2.78613   0.4699   L
 O-OW--0.834000       0    -10.30353  -2.13103   11.55014  L
 H-HW-0.417000        0    -10.61282  -1.28356   11.14919  L
 H-HW-0.417000        0    -10.587   -2.78327   10.88496  L
 O-OW--0.834000       0    -10.27651  -3.88517   9.46945  L
 H-HW-0.417000        0    -10.52931  -3.23759   8.78397  L
 H-HW-0.417000        0    -9.63898  -4.44847   8.98981  L
 O-OW--0.834000       0    -10.72028  -1.97007   7.6314   L
 H-HW-0.417000        0    -11.51743  -1.5645    8.05849  L
 H-HW-0.417000        0    -10.07995  -1.25462   7.71062  L
 O-OW--0.834000       0     5.44416   3.97443   1.76509  H
 H-HW-0.417000        0     4.76632   4.34355   2.40607  H
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H-HW-0.417000        0     5.02297   2.53854   1.62389  H
O-OW--0.834000       0     6.99959   4.93088   3.92781  H
H-HW-0.417000        0     6.72229   4.44342   3.12813  H
H-HW-0.417000        0     6.52073   5.76053   3.71468  H
O-OW--0.834000       0     6.40139   2.33134  -5.36899  L
H-HW-0.417000        0     7.25007   2.10338  -5.79411  L
H-HW-0.417000        0     6.137     3.14461  -5.82259  L
O-OW--0.834000       0     6.48299   5.58859   6.57506  L
H-HW-0.417000        0     5.68179   5.08383   6.79916  L
H-HW-0.417000        0     6.70091   5.25455   5.68586  L
O-OW--0.834000       0     7.82898   1.57915   5.49078  H
H-HW-0.417000        0     7.16967   2.26023   5.28501  H
H-HW-0.417000        0     7.20952   0.82918   5.72191  H
O-OW--0.834000       0     5.55966   7.08279   2.47375  H
H-HW-0.417000        0     4.79922   7.6919    2.42847  H
H-HW-0.417000        0     5.8562    7.12431   1.54673  H
O-OW--0.834000       0     3.70089   16.44976   3.61135  L
H-HW-0.417000        0     3.3488    15.58229   3.35789  L
H-HW-0.417000        0     2.93015   17.01757   3.58011  L
O-OW--0.834000       0    -4.33329   2.09102   5.59327  L
H-HW-0.417000        0    -4.12712   2.0562    6.53211  L
H-HW-0.417000        0    -4.82731   2.95321   5.53349  L
O-OW--0.834000       0     0.259     1.82158   12.14841  L
H-HW-0.417000        0    -0.12237   1.60464   13.0221  L
H-HW-0.417000        0     0.03512   2.75246   12.07085  L
O-OW--0.834000       0    -2.22046   9.76227   5.72575  L
H-HW-0.417000        0    -2.07066   8.8583    6.06842  L
H-HW-0.417000        0    -1.7043    9.787     4.88695  L
O-OW--0.834000       0     2.22349   9.14443   6.68569  L
H-HW-0.417000        0     1.72897   8.43175   6.24384  L
H-HW-0.417000        0     1.59078   9.89225   6.62241  L
O-OW--0.834000       0    -4.85908   9.00517   5.58435  L
H-HW-0.417000        0    -4.77764   8.11044   5.96994  L
H-HW-0.417000        0    -3.96846   9.38033   5.70605  L
O-OW--0.834000       0    -2.33811   7.31      6.97041  L
H-HW-0.417000        0    -3.20473   6.88617   6.77418  L
H-HW-0.417000        0    -2.14509   7.01069   7.87478  L
O-OW--0.834000       0     0.24458   10.89595   6.19428  L
H-HW-0.417000        0     0.30179   10.91874   5.22246  L
H-HW-0.417000        0    -0.6862    10.64975   6.32504  L
O-O2--0.818800       0     5.93801   7.87358  -0.29988  H
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**TS2**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.52118 | -11.69758 | -5.5696 | L |
| C-C-0.597200 | 0 | -11.84375 | -10.67628 | -6.45401 | L |
| O-O--0.567900 | 0 | -11.45868 | -11.0201 | -7.56263 | L |
| H-HC-0.112300 | 0 | -11.91327 | -11.85647 | -4.68181 | L |
| H-HC-0.112300 | 0 | -12.60856 | -12.63164 | -6.12246 | L |
| H-HC-0.112300 | 0 | -13.51162 | -11.33632 | -5.30186 | L |
| N-N--0.415700 | 0 | -11.66826 | -9.45521 | -5.93988 | L |
| C-CT--0.058100 | -1 | -10.80971 | -8.42136 | -6.53771 | L |
| C-C-0.597300 | 0 | -9.78603 | -7.90463 | -5.52111 | L |
| O-O--0.567900 | 0 | -10.06241 | -7.83765 | -4.3169 | L |
| C-CT--0.007400 | 0 | -11.62117 | -7.31912 | -7.21361 | L |
| C-CC-0.186800 | 0 | -11.02702 | -6.8289 | -8.50808 | L |
| N-NB--0.543200 | 0 | -11.43652 | -7.22051 | -9.78224 | L |
| C-CW--0.220700 | 0 | -10.14945 | -5.79357 | -8.61977 | L |
| C-CR-0.163500 | 0 | -10.84862 | -6.36304 | -10.62952 | L |
| N-NA--0.279500 | 0 | -10.07329 | -5.49464 | -9.9613 | L |
| H-H-0.271900 | 0 | -12.03789 | -9.25964 | -5.02552 | L |
| H-H1-0.136000 | 0 | -10.23986 | -8.90564 | -7.33278 | L |
| H-HC-0.036700 | 0 | -11.68152 | -6.47389 | -6.53782 | L |
| H-HC-0.036700 | 0 | -12.6314 | -7.67377 | -7.42272 | L |
| H-H4-0.186200 | 0 | -9.71229 | -5.22967 | -7.81108 | L |
| H-H-0.333900 | 0 | -9.71758 | -4.61632 | -10.35863 | L |
| H-H5-0.143500 | 0 | -11.03539 | -6.32333 | -11.69324 | L |
| N-N--0.415700 | 0 | -8.59433 | -7.5644 | -6.00619 | L |
| C-CT--0.038900 | -1 | -7.4395 | -7.05855 | -5.24287 | L |
| C-C-0.597300 | 0 | -6.66874 | -5.9735 | -6.03095 | L |
| O-O--0.567900 | 0 | -7.01913 | -5.65706 | -7.16739 | L |
| C-CT-0.365400 | 0 | -6.44685 | -8.18667 | -4.89049 | L |
| O-OH--0.676100 | 0 | -6.16012 | -8.96358 | -6.01459 | L |
| C-CT--0.243800 | -1 | -6.95643 | -9.13608 | -3.82466 | L |
| H-H-0.271900 | 0 | -8.43825 | -7.75685 | -6.98977 | L |
| H-H1-0.100700 | 0 | -7.7755 | -6.62724 | -4.30706 | L |
| H-H1-0.004300 | 0 | -5.51821 | -7.75457 | -4.51766 | L |
| H-HC-0.064200 | 0 | -7.23381 | -8.57466 | -2.93242 | L |
| H-HC-0.064200 | 0 | -6.17539 | -9.8496 | -3.56659 | L |
| H-HC-0.064200 | 0 | -7.82974 | -9.67394 | -4.19457 | L |
| H-HO-0.410200 | 0 | -5.44387 | -9.58555 | -5.80749 | L |
| N-N--0.347900 | 0 | -5.59265 | -5.39646 | -5.4595 | L |
| C-CT--0.263700 | -1 | -4.61403 | -4.53686 | -6.17421 | L |
| C-C-0.734100 | 0 | -3.21088 | -4.58951 | -5.57947 | L |
| O-O--0.589400 | 0 | -3.09457 | -4.80154 | -4.37763 | L |
| C-CT--0.000700 | 0 | -5.13827 | -3.08583 | -6.28732 | L |
| C-CT-0.039000 | 0 | -4.95377 | -2.14228 | -5.07996 | L |
| C-CT-0.048600 | 0 | -5.72948 | -2.46437 | -3.79784 | L |
| N-N2--0.529500 | 0 | -5.10579 | -3.52112 | -2.99209 | L |
| C-CA-0.807600 | 0 | -5.04967 | -3.60264 | -1.6811 | L |
| N-N2--0.862700 | 0 | -5.70585 | -2.82448 | -0.87445 | L |
| N-N2--0.862700 | 0 | -4.28529 | -4.50735 | -1.1554 | L |
| H-H-0.274700 | 0 | -5.35561 | -5.70767 | -4.52966 | L |
| H-H1-0.156000 | 0 | -4.5477 | -4.94066 | -7.18059 | L |

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 H-HC-0.032700        0    -6.19433  -3.10259  -6.56032  L
 H-HC-0.032700        0    -4.61528  -2.62184  -7.12518  L
 H-HC-0.028500        0    -5.30328  -1.16102  -5.39357  L
 H-HC-0.028500        0    -3.89507  -2.04413  -4.84859  L
 H-H1-0.068700        0    -6.75264  -2.73033  -4.05662  L
 H-H1-0.068700        0    -5.7464   -1.55106  -3.20213  L
 H-H-0.345600         0    -4.46896  -4.13786  -3.47342  L
 H-H-0.447800         0    -5.72076  -2.9527    0.12568  L
 H-H-0.447800         0    -6.42156  -2.19454  -1.26139  L
 H-H-0.447800         0    -3.98628  -4.37427  -0.1958   L
 H-H-0.447800         0    -3.85395  -5.21044  -1.74774  L
 N-N--0.415700        0    -2.15381  -4.3089   -6.3381   L
 C-CT--0.002400      -1    -0.92333  -3.76165  -5.73887  L
 C-C-0.597300         0    -1.08275  -2.22831  -5.5963   L
 O-O--0.567900        0    -1.3682   -1.59328  -6.61302  L
 C-CT--0.034300       0     0.30826  -4.1215   -6.57539  L
 C-CA-0.011800        0     1.59689  -3.54089  -6.01403  L
 C-CA--0.125600       0     2.05199  -3.90894  -4.73073  L
 C-CA--0.125600       0     2.33578  -2.61037  -6.76712  L
 C-CA--0.170400       0     3.22414  -3.33235  -4.20595  L
 C-CA--0.170400       0     3.50938  -2.0422   -6.24719  L
 C-CA--0.107200       0     3.94228  -2.38651  -4.95812  L
 H-H-0.271900         0    -2.34514  -4.15631  -7.32428  L
 H-H1-0.097800        0    -0.77003  -4.21123  -4.76078  L
 H-HC-0.029500        0     0.16093  -3.76743  -7.59727  L
 H-HC-0.029500        0     0.40566  -5.20709  -6.60388  L
 H-HA-0.133000        0     1.49889  -4.6256   -4.14046  L
 H-HA-0.133000        0     1.99767  -2.31248  -7.74519  L
 H-HA-0.143000        0     3.57124  -3.60375  -3.22033  L
 H-HA-0.143000        0     4.0636   -1.31923  -6.82933  L
 H-HA-0.129700        0     4.82292  -1.90953  -4.55244  L
 N-N--0.254800        0    -0.96725  -1.63943  -4.38296  L
 C-CT--0.026600       0    -1.14594  -0.20191  -4.14037  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.16224   0.51296  -3.69027  H
 O-O--0.574800        0     0.54996   0.49716  -2.53103  H
 C-CT--0.007000       0    -2.18826  -0.17588  -3.02097  L
 C-CT-0.018900        0    -1.79943  -1.36811  -2.14693  L
 C-CT-0.019200        0    -1.10398  -2.33644  -3.10534  L
 H-H1-0.064100        0    -1.55553   0.31249  -5.00809  L
 H-HC-0.025300        0    -3.18275  -0.33051  -3.43767  L
 H-HC-0.025300        0    -2.15581   0.74906  -2.45227  L
 H-HC-0.021300        0    -2.67635  -1.81889  -1.68267  L
 H-HC-0.021300        0    -1.09526  -1.05009  -1.38341  L
 H-H1-0.039100        0    -0.123    -2.61025  -2.71715  L
 H-H1-0.039100        0    -1.72605  -3.22149  -3.19571  L
 N-N--0.254800        0     0.85745   1.20105  -4.63701  H
 C-CT--0.026600       0     2.07904   1.9091   -4.31204  H
 C-C-0.589600         0     1.93393   3.4219   -4.51726  H
 O-O--0.574800        0     1.20283   3.87825  -5.38258  H
 C-CT--0.007000       0     3.03562   1.44199  -5.42615  H
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 C-CT-0.018900        0     2.11782   1.36125  -6.65969  H
 C-CT-0.019200        0     0.69766   1.13298  -6.09219  H
 H-H1-0.064100        0     2.41304   1.66823  -3.3003   H
 H-HC-0.025300        0     3.44603   0.46973  -5.15072  H
 H-HC-0.025300        0     3.86707   2.13729  -5.57223  H
 H-HC-0.021300        0     2.41645   0.56156  -7.3388   H
 H-HC-0.021300        0     2.14041   2.30216  -7.21133  H
 H-H1-0.039100        0     0.01811   1.92128  -6.41045  H
 H-H1-0.039100        0     0.30416   0.16117  -6.38935  H
 N-N--0.415700        0     2.78538   4.13051  -3.73336  H
 C-CT-0.039700        0     3.19668   5.52363  -3.89413  H
 C-C-0.597300         0     4.15158   5.65213  -5.13991  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.22147   5.03492  -5.11505  L
 C-CT--0.003600       0     3.73667   5.91566  -2.47843  H
 C-CT-0.013600        0     4.93225   6.85544  -2.33797  H
 C-C-0.805400         0     5.44919   6.87534  -0.9022   H
 O-O2--0.818800       0     5.77478   5.85343  -0.30033  H
 H-H-0.271900         0     3.13844   3.65741  -2.9145   H
 H-H1-0.110500        0     2.32216   6.14701  -4.10388  H
 H-HC--0.017300       0     2.89179   6.3113   -1.91226  H
 H-HC--0.017300       0     3.99872   5.00837  -1.92202  H
 H-HC--0.042500       0     4.72819   7.87341  -2.67293  H
 H-HC--0.042500       0     5.77733   6.48775  -2.93047  H
 N-N--0.254800        0     3.78771   6.3418   -6.26239  L
 C-CT--0.026600       -1    4.64665   6.66129  -7.44538  L
 C-C-0.589600         0     6.07911   7.11096  -7.1139   L
 O-O--0.574800        0     6.98163   6.91887  -7.93034  L
 C-CT--0.007000       0     3.86773   7.67475  -8.26698  L
 C-CT-0.018900        0     2.42359   7.28617  -7.98712  L
 C-CT-0.019200        0     2.44317   6.85469  -6.52114  L
 H-H1-0.064100        0     4.72674   5.7517   -8.03723  L
 H-HC-0.025300        0     4.11106   7.62119  -9.32848  L
 H-HC-0.025300        0     4.04998   8.66332  -7.87183  L
 H-HC-0.021300        0     2.14437   6.44227  -8.61599  L
 H-HC-0.021300        0     1.75527   8.12513  -8.1554   L
 H-H1-0.039100        0     2.23323   7.71218  -5.88254  L
 H-H1-0.039100        0     1.68552   6.09157  -6.35808  L
 N-N--0.415700        0     6.3293    7.6707   -5.92627  L
 C-CT-0.014300        -1    7.67265   7.88323  -5.40209  L
 C-C-0.597300         0     8.48303   6.59511  -5.27966  L
 O-O--0.567900        0     8.32831   5.80046  -4.35092  L
 C-CT--0.204100       0     7.65617   8.64482  -4.06087  L
 C-C-0.713000         0     9.05646   9.0115   -3.58533  L
 O-O--0.593100        0     9.66931   8.37103  -2.74177  L
 N-N--0.919100        0     9.63659   10.05734  -4.11861  L
 H-H-0.271900         0     5.51478   7.92741  -5.36686  L
 H-H1-0.104800        0     8.18546   8.52742  -6.11823  L
 H-HC-0.079700        0     7.20397   8.03517  -3.28846  L
 H-HC-0.079700        0     7.06762   9.54829  -4.16684  L
 H-H-0.419600         0     10.5442   10.28666  -3.76589  L
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H-H-0.419600          0     9.14595   10.65633  -4.78047  L
N-N--0.415700         0     9.45026   6.46864   -6.17718  L
C-CT--0.025200        -1    10.67327   5.7526    -5.89479  L
C-C-0.597300          0     11.03781   4.74319  -6.98924  L
O-O--0.567900         0     11.5305   5.10013   -8.05527  L
H-H-0.271900          0     9.40522   7.05979   -6.99532  L
H-H1-0.069800         0     10.61143   5.2362    -4.93632  L
H-H1-0.069800         0     11.48726   6.4739    -5.82746  L
N-N--0.415700         0     10.80942   3.47142   -6.6804   L
C-CT--0.001400        -1    10.82053   2.28631   -7.55107  L
C-C-0.597300          0     9.75967   1.34824   -6.94997  L
O-O--0.567900         0     8.92274   1.79306   -6.15638  L
C-CT--0.015200        0     12.24956   1.70443   -7.60856  L
C-CA--0.001100        0     12.67617   1.29728   -9.00506  L
C-CA--0.190600        0     13.03739   2.29848   -9.92802  L
C-CA--0.190600        0     12.71436  -0.058     -9.38754  L
C-CA--0.234100        0     13.43482   1.95139   -11.23341  L
C-CA--0.234100        0     13.1033  -0.40894   -10.69486  L
C-C-0.322600          0     13.46326   0.59346   -11.61883  L
O-OH--0.557900        0     13.8368   0.25039   -12.87916  L
H-H-0.271900          0     10.31228   3.33333   -5.81194  L
H-H1-0.087600         0     10.5006   2.57726   -8.55266  L
H-HC-0.029500         0     12.35109   0.86288   -6.92259  L
H-HC-0.029500         0     12.96046   2.46064   -7.27097  L
H-HA-0.169900         0     12.9962   3.33923   -9.62921  L
H-HA-0.169900         0     12.44652  -0.83527   -8.68689  L
H-HA-0.165600         0     13.70576   2.72511   -11.93418  L
H-HA-0.165600         0     13.12693  -1.44212   -11.00579  L
H-HO-0.399200         0     14.04832   1.02438   -13.40053  L
N-N--0.415700         0     9.84844   0.04875   -7.18704  L
C-CT--0.051800        -1    9.40981  -0.94279   -6.20502  L
C-C-0.597300          0     10.58826  -1.83987   -5.87268  L
O-O--0.567900         0     11.57302  -1.92139   -6.60716  L
C-CT--0.110200        0     8.16295  -1.68004   -6.74115  L
C-CT-0.353100         0     8.38042  -2.57919   -7.97839  L
C-CT--0.412100        0     8.80159  -4.00485   -7.60002  L
C-CT--0.412100        0     7.07354  -2.6888    -8.76239  L
H-H-0.271900          0     10.50399  -0.24665   -7.89797  L
H-H1-0.092200         0     9.14184  -0.41943   -5.29377  L
H-HC-0.045700         0     7.4261   -0.91295   -6.98617  L
H-HC-0.045700         0     7.72903  -2.28529   -5.94713  L
H-HC--0.036100        0     9.1342   -2.14426   -8.63434  L
H-HC-0.100000         0     9.78521  -4.00251   -7.13776  L
H-HC-0.100000         0     8.85576  -4.6182    -8.49933  L
H-HC-0.100000         0     8.07865  -4.44198   -6.91189  L
H-HC-0.100000         0     6.27828  -3.07376   -8.12934  L
H-HC-0.100000         0     7.20545  -3.33649   -9.6295   L
H-HC-0.100000         0     6.78671  -1.70395   -9.11569  L
N-N--0.415700         0     10.50196  -2.49207   -4.72928  L
C-CT--0.058100        -1    11.58816  -3.28772   -4.17727  L
C-C-0.597300          0     11.09446  -4.68772   -3.83619  L
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 O-O--0.567900        0     9.90045  -4.97494  -3.85817  L
 C-CT--0.007400       0     12.16092  -2.53692  -2.95999  L
 C-CC-0.186800        0     11.14011  -2.19046  -1.89647  L
 N-NB--0.543200       0     10.72424  -3.0252   -0.85894  L
 C-CW--0.220700       0     10.42518  -1.03031  -1.83939  L
 C-CR-0.163500        0     9.7723   -2.34496  -0.19624  L
 N-NA--0.279500       0     9.55958  -1.1525   -0.77342  L
 H-H-0.271900         0     9.64098  -2.38781  -4.20353  L
 H-H1-0.136000        0     12.38167  -3.40079  -4.91794  L
 H-HC-0.036700        0     12.61234  -1.60806  -3.31151  L
 H-HC-0.036700        0     12.95614  -3.12877  -2.51282  L
 H-H4-0.186200        0     10.4841  -0.21133  -2.54313  L
 H-H-0.333900         0     8.8032   -0.52193  -0.53065  L
 H-H5-0.143500        0     9.21198  -2.71695   0.65243  L
 N-N--0.415700        0     12.00877  -5.59792  -3.51905  L
 C-CT--0.059700       -1    11.61578  -6.97399  -3.21315  L
 C-C-0.597300         0     10.69416  -7.10326  -1.97479  L
 O-O--0.567900        0     9.93332  -8.06345  -1.86954  L
 C-CT-0.130300        0     12.85086  -7.88558  -3.11357  L
 C-CT--0.043000       0     12.39256  -9.35677  -3.03345  L
 C-CT--0.320400       0     13.77219  -7.50583  -1.93902  L
 C-CT--0.066000       -1    13.45957  -10.33303  -3.50707  L
 H-H-0.271900         0     12.98492  -5.34743  -3.53549  L
 H-H1-0.086900        0     11.03538  -7.32718  -4.06321  L
 H-HC-0.018700        0     13.41585  -7.75808  -4.03913  L
 H-HC-0.023600        0     11.52327  -9.50408  -3.67516  L
 H-HC-0.023600        0     12.10946  -9.60847  -2.01049  L
 H-HC-0.088200        0     14.67517  -8.11224  -1.97213  L
 H-HC-0.088200        0     13.27146  -7.67384  -0.98482  L
 H-HC-0.088200        0     14.07308  -6.4614   -2.00495  L
 H-HC-0.018600        0     13.0655  -11.34855  -3.45902  L
 H-HC-0.018600        0     14.34123  -10.26898  -2.86976  L
 H-HC-0.018600        0     13.73879  -10.11093  -4.53763  L
 N-N--0.415700        0     10.70624  -6.13035  -1.05663  L
 C-CT--0.025200       -1    9.682    -6.00072  -0.01895  L
 C-C-0.597300         0     8.28713  -5.88389  -0.63146  L
 O-O--0.567900        0     7.47154  -6.79732  -0.49128  L
 H-H-0.271900         0     11.32199  -5.34335  -1.19869  L
 H-H1-0.069800        0     9.88564  -5.1287    0.59793  L
 H-H1-0.069800        0     9.70162  -6.88518   0.61291  L
 N-N--0.415700        0     8.04113  -4.80076  -1.38014  L
 C-CT--0.058100       0     6.84549  -4.62862  -2.2208   L    H-HC
246   0.        0.
 C-C-0.597300         0     6.49845  -5.89917  -3.00814  L
 O-O--0.567900        0     5.3288   -6.26932  -3.07642  L
 C-CT--0.007400       0     7.03198  -3.48115  -3.21615  H
 C-CC-0.186800        0     7.02258  -2.05906  -2.75945  H
 N-NB--0.543200       0     7.71022  -1.15744  -3.53149  H
 C-CW--0.220700       0     6.25915  -1.39436  -1.83702  H
 C-CR-0.163500        0     7.31248   0.02841  -3.13059  H
 N-NA--0.279500       0     6.45223  -0.0562   -2.08632  H
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H-H-0.271900          0     8.80184  -4.14076  -1.49276  L
H-H1-0.136000         0     5.98595  -4.4023   -1.58671  L
H-HC-0.036700         0     6.23427  -3.58436  -3.96106  H
H-HC-0.036700         0     7.95097  -3.63049  -3.77582  H
H-H4-0.186200         0     5.58533  -1.70856  -1.06399  H
H-H-0.333900          0     5.85809   0.70893  -1.76251  H
H-H5-0.143500         0     7.61973   0.98298  -3.55112  H
N-N--0.415700         0     7.49583  -6.58574  -3.57815  L
C-CT-0.033700         -1    7.30799  -7.83351  -4.31527  L
C-C-0.597300          0     6.50543  -8.90701  -3.57518  L
O-O--0.567900         0     5.68232  -9.57704  -4.19847  L
C-CT--0.182500        0     8.62667  -8.35976  -4.88635  L
H-H-0.271900          0     8.42155  -6.1741   -3.53175  L
H-H1-0.082300         0     6.69724  -7.57285  -5.17813  L
H-HC-0.060300         0     9.17165  -7.54977  -5.37252  L
H-HC-0.060300         0     8.41167  -9.12915  -5.62915  L
H-HC-0.060300         0     9.22956  -8.8077   -4.10191  L
N-N--0.347900         0     6.67277  -9.05401  -2.25612  L
C-CT--0.240000        -1    5.78775  -9.91738  -1.4638   L
C-C-0.734100          0     4.31064  -9.46887  -1.52393  L
O-O--0.589400         0     3.43818  -10.31718  -1.68915  L
C-CT--0.009400        0     6.30066  -10.05471  -0.02036  L
C-CT-0.018700         0     5.42028  -11.01323   0.80753  L
C-CT--0.047900        0     6.04545  -11.31551   2.17329  L
C-CT--0.014300        0     5.08367  -12.09555   3.07753  L
N-N3--0.385400        0     5.66684  -12.30439   4.42769  L
H-H-0.274700          0     7.3494   -8.44485  -1.80108  L
H-H1-0.142600         0     5.80725  -10.9098  -1.91767  L
H-HC-0.036200         0     6.31751  -9.07503   0.45806  L
H-HC-0.036200         0     7.3205   -10.44207  -0.0522   L
H-HC-0.010300         0     5.28706  -11.95021   0.26435  L
H-HC-0.010300         0     4.44299  -10.55524   0.96409  L
H-HC-0.062100         0     6.28713  -10.36779   2.65273  L
H-HC-0.062100         0     6.95858  -11.89405   2.02602  L
H-HP-0.113500         0     4.83091  -13.05121   2.60949  L
H-HP-0.113500         0     4.16335  -11.50898   3.17346  L
H-H-0.340000          0     4.94815  -12.56769   5.09784  L
H-H-0.340000          0     6.02183  -11.41476   4.77916  L
H-H-0.340000          0     6.41895  -12.97487   4.42636  L
N-N--0.415700         0     4.01992  -8.16963  -1.38619  L
C-CT--0.024900        -1    2.66866  -7.5928   -1.56131  L
C-C-0.597300          0     2.11585  -7.85856  -2.97192  L
O-O--0.567900         0     0.99098  -8.34118  -3.07356  L
C-CT-0.211700         0     2.6587   -6.08812  -1.23232  L
O-OH--0.654600        0     1.32491  -5.62529  -1.12929  L
H-H-0.271900          0     4.80736  -7.5362   -1.33803  L
H-H1-0.084300         0     1.99842  -8.08549  -0.85623  L
H-H1-0.035200         0     3.17997  -5.52801  -2.00718  L
H-H1-0.035200         0     3.16256  -5.92602  -0.2794   L
H-HO-0.427500         0     1.30525  -4.69663  -0.83224  L
N-N--0.415700         0     2.89183  -7.62674  -4.0477   L
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C-CT--0.059700       -1    2.56575  -8.04651  -5.43764  L
C-C-0.597300         0     2.15633  -9.53716  -5.42311  L
O-O--0.567900        0     1.03106  -9.85692  -5.78649  L
C-CT-0.130300        0     3.71562  -7.7436   -6.42813  L
C-CT--0.043000       0     4.04164  -6.23395  -6.43286  L
C-CT--0.320400       0     3.34427  -8.20352  -7.85012  L
C-CT--0.066000       0     5.27038  -5.84942  -7.26123  L
H-H-0.271900         0     3.79234  -7.19364  -3.8689   L
H-H1-0.086900        0     1.69081  -7.48159  -5.76194  L
H-HC-0.018700        0     4.60298  -8.291    -6.11622  L
H-HC-0.023600        0     4.23297  -5.89987  -5.41558  L
H-HC-0.023600        0     3.18188  -5.68133  -6.81051  L
H-HC-0.088200        0     2.49501  -7.6298   -8.22311  L
H-HC-0.088200        0     3.09179  -9.26387  -7.86626  L
H-HC-0.088200        0     4.18685  -8.06016  -8.52594  L
H-HC-0.018600        0     5.04569  -5.90888  -8.32613  L
H-HC-0.018600        0     6.10997  -6.50239  -7.02817  L
H-HC-0.018600        0     5.54211  -4.82558  -7.01416  L
N-N--0.415700        0     3.01889  -10.44752  -4.95287  L
C-CT-0.021300        -1    2.79565  -11.9063  -4.96412  L
C-C-0.597300         0     1.57304  -12.41381  -4.20107  L
O-O--0.567900        0     1.02317  -13.44929  -4.56174  L
C-CT--0.123100       -1    4.10586  -12.64414  -4.55279  L
S-SH--0.311900       0     5.4499   -12.29959  -5.72487  L
H-H-0.271900         0     3.9225   -10.11012  -4.64433  L
H-H1-0.112400        0     2.59883  -12.18508  -6.00129  L
H-H1-0.111200        0     3.91257  -13.71883  -4.55082  L
H-H1-0.111200        0     4.39891  -12.33733  -3.54796  L
H-HS-0.193300        0     5.61151  -11.00764  -5.40155  L
N-N--0.415700        0     1.14457  -11.7126  -3.15604  L
C-CT--0.051800       -1   -0.08879  -12.0273  -2.44098  L
C-C-0.597300         0    -1.32003  -11.38283  -3.10409  L
O-O--0.567900        0    -2.29494  -12.08757  -3.34026  L
C-CT--0.110200       0     0.05624  -11.56039  -0.98128  L
C-CT-0.353100        0     1.07571  -12.3887  -0.17491  L
C-CT--0.412100       0     1.41955  -11.66578   1.12534  L
C-CT--0.412100       0     0.53667  -13.77481   0.18611  L
H-H-0.271900         0     1.68632  -10.89944  -2.89028  L
H-H1-0.092200        0    -0.25844  -13.10469  -2.45413  L
H-HC-0.045700        0    -0.9151   -11.62382  -0.48846  L
H-HC-0.045700        0     0.361    -10.51204  -0.98132  L
H-HC--0.036100       0     1.99766  -12.50987  -0.7427   L
H-HC-0.100000        0     1.86528  -10.703    0.87955  L
H-HC-0.100000        0     2.1293   -12.25384   1.70238  L
H-HC-0.100000        0     0.51401  -11.50002   1.71085  L
H-HC-0.100000        0     1.27061  -14.3172   0.77978  L
H-HC-0.100000        0     0.34208  -14.34558  -0.72155  L
H-HC-0.100000        0    -0.39096  -13.68099   0.75162  L
N-N--0.415700        0    -1.29553  -10.07962  -3.42587  L
C-CT-0.014300        -1   -2.39573  -9.38642  -4.12511  L
C-C-0.597300         0    -2.75213  -10.07177  -5.42978  L
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O-O--0.567900        0    -3.90015  -10.46872  -5.63287  L
C-CT--0.204100       0    -2.12488  -7.8822   -4.23702  L
C-C-0.713000         0    -2.33844  -7.19083  -2.89906  L
O-O--0.593100        0    -3.45085  -6.8889   -2.49178  L
N-N--0.919100        0    -1.29073  -6.91997  -2.16123  L
H-H-0.271900         0    -0.44151  -9.56515  -3.24452  L
H-H1-0.104800        0    -3.28987  -9.49901  -3.50681  L
H-HC-0.079700        0    -2.8385   -7.45358  -4.93902  L
H-HC-0.079700        0    -1.12087  -7.6946   -4.61518  L
H-H-0.419600         0    -1.42401  -6.41365  -1.3065   L
H-H-0.419600         0    -0.36956  -7.19929  -2.47075  L
N-N--0.415700        0    -1.73879  -10.29553  -6.25486  L
C-CT--0.002400       -1   -1.87777  -11.11321  -7.43841  L
C-C-0.597300         0    -2.06424  -12.60901  -7.19831  L
O-O--0.567900        0    -2.54646  -13.31525  -8.07821  L
C-CT--0.034300       0    -0.74278  -10.8208  -8.43567  L
C-CA-0.011800        0    -0.87876  -9.46833  -9.11979  L
C-CA--0.125600       0    -1.61065  -9.36465  -10.31872  L
C-CA--0.125600       0    -0.33239  -8.30472  -8.54337  L
C-CA--0.170400       0    -1.80992  -8.11041  -10.92372  L
C-CA--0.170400       0    -0.52227  -7.05117  -9.15464  L
C-CA--0.107200       0    -1.26932  -6.95246  -10.34037  L
H-H-0.271900         0    -0.81561  -9.95692  -6.00971  L
H-H1-0.097800        0    -2.79858  -10.80418  -7.93643  L
H-HC-0.029500        0    -0.75821  -11.58671  -9.21252  L
H-HC-0.029500        0     0.22393  -10.89646  -7.94069  L
H-HA-0.133000        0    -2.05144  -10.24534  -10.76359  L
H-HA-0.133000        0     0.21233  -8.36703  -7.61686  L
H-HA-0.143000        0    -2.40429  -8.02857  -11.82437  L
H-HA-0.143000        0    -0.11795  -6.15573  -8.70887  L
H-HA-0.129700        0    -1.44451  -5.98708  -10.79657  L
N-N--0.415700        0    -1.72782  -13.08416  -6.00531  L
C-CT--0.025200       -1   -1.93761  -14.45703  -5.57799  L
C-C-0.597300         0    -3.39687  -14.87487  -5.43393  L
O-O--0.567900        0    -3.74809  -16.01069  -5.73941  L
H-H-0.271900         0    -1.35959  -12.43644  -5.32764  L
H-H1-0.069800        0    -1.44957  -14.60611  -4.61569  L
H-H1-0.069800        0    -1.46809  -15.12605  -6.29958  L
N-N--0.415700        0    -4.23448  -13.96693  -4.93534  L
C-CT--0.059700       -1   -5.69416  -14.12823  -4.87211  L
C-C-0.597300         0    -6.35697  -14.0874  -6.25241  L
O-O--0.567900        0    -7.36839  -14.75539  -6.46139  L
C-CT-0.130300        0    -6.25496  -13.08477  -3.84993  L
C-CT--0.043000       0    -5.92713  -13.57392  -2.39884  L
C-CT--0.320400       -1   -7.77122  -12.76504  -4.00273  L
C-CT--0.066000       -1   -5.24924  -12.56516  -1.44169  L
H-H-0.271900         0    -3.82516  -13.08563  -4.64879  L
H-H1-0.086900        0    -5.91558  -15.12434  -4.48685  L
H-HC-0.018700        0    -5.72365  -12.14693  -4.02057  L
H-HC-0.023600        0    -5.26294  -14.43777  -2.44617  L
H-HC-0.023600        0    -6.84606  -13.92518  -1.92774  L
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H-HC-0.088200        0    -7.95782  -12.2881  -4.96705  L
H-HC-0.088200        0    -8.08662  -12.08101  -3.21495  L
H-HC-0.088200        0    -8.35494  -13.68432  -3.94336  L
H-HC-0.018600        0    -4.29749  -12.24022  -1.85251  L
H-HC-0.018600        0    -5.0806   -13.03502  -0.47263  L
H-HC-0.018600        0    -5.89668  -11.69762  -1.31335  L
N-N--0.415700        0    -5.76538  -13.35111  -7.19622  L
C-CT--0.149000       -1   -6.16526  -13.34675  -8.59168  L
H-H-0.271900         0    -4.92977  -12.85426  -6.93009  L
H-H1-0.097600        0    -6.43849  -14.35649  -8.90362  L
H-H1-0.097600        0    -5.34063  -12.99085  -9.2105   L
H-H1-0.097600        0    -7.02809  -12.68932  -8.71997  L
C-CT--0.366200       -1   -8.60726  -10.21468  -10.75209  L
C-C-0.597200         0    -7.85868  -9.52838  -9.67555  L
O-O--0.567900        0    -8.21083  -9.55081  -8.5038   L
H-HC-0.112300        0    -7.96618  -10.93514  -11.25441  L
H-HC-0.112300        0    -8.99271  -9.47404  -11.45113  L
H-HC-0.112300        0    -9.45195  -10.73311  -10.29682  L
N-N--0.415700        0    -6.79953  -8.90294  -10.13277  L
C-CT-0.021300        -1   -6.01079  -8.02767  -9.32449  L
C-C-0.597300         0    -5.52192  -6.86872  -10.19222  L
O-O--0.567900        0    -4.92272  -7.11822  -11.24187  L
C-CT--0.123100       0    -4.80666  -8.80918  -8.7772   L
S-SH--0.311900       0    -3.73461  -7.71374  -7.79051  L
H-H-0.271900         0    -6.61509  -8.91691  -11.12298  L
H-H1-0.112400        0    -6.6008   -7.64242  -8.49392  L
H-H1-0.111200        0    -4.23569  -9.2207   -9.60889  L
H-H1-0.111200        0    -5.16511  -9.63478  -8.16207  L
H-HS-0.193300        0    -3.25734  -6.99546  -8.82047  L
N-N--0.415700        0    -5.74255  -5.62447  -9.76523  L
C-CT-0.014300        -1   -5.28638  -4.45616  -10.51379  L
C-C-0.597300         0    -3.91043  -3.90926  -10.03374  L
O-O--0.567900        0    -3.33541  -4.36124  -9.03907  L
C-CT--0.204100       0    -6.41357  -3.40695  -10.59616  L
C-C-0.713000         0    -6.23433  -2.42031  -11.74872  L
O-O--0.593100        0    -5.40029  -2.5976   -12.62676  L
N-N--0.919100        0    -6.96013  -1.33709  -11.78275  L
H-H-0.271900         0    -6.26523  -5.49389  -8.90411  L
H-H1-0.104800        0    -5.11554  -4.78113  -11.54185  L
H-HC-0.079700        0    -6.49474  -2.86047  -9.65706  L
H-HC-0.079700        0    -7.35029  -3.92926  -10.77662  L
H-H-0.419600         0    -6.83013  -0.72272  -12.55738  L
H-H-0.419600         0    -7.75886  -1.21381  -11.14563  L
N-N--0.415700        0    -3.35516  -2.92513  -10.7433  L
C-CT--0.051800       -1   -2.23151  -2.08013  -10.33158  L
C-C-0.597300         0    -2.79326  -0.65847  -10.05583  L
O-O--0.567900        0    -3.0416    0.08994  -11.00013  L
C-CT--0.110200       0    -1.15005  -2.09874  -11.42971  L
C-CT-0.353100        0     0.01463  -1.11371  -11.20048  L
C-CT--0.412100       0     0.75996  -1.39167  -9.89647  L
C-CT--0.412100       0     1.02466  -1.24193  -12.34363  L
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H-H-0.271900          0    -3.87621  -2.62222  -11.56297  L
H-H1-0.092200         0    -1.79828  -2.45849  -9.40539  L
H-HC-0.045700         0    -1.62164  -1.84753  -12.38153  L
H-HC-0.045700         0    -0.75397  -3.11185  -11.50725  L
H-HC--0.036100        0    -0.35547  -0.09052  -11.18479  L
H-HC-0.100000         0     1.10343  -2.42478  -9.87925  L
H-HC-0.100000         0     0.09943  -1.20064  -9.04965  L
H-HC-0.100000         0     1.60646  -0.71169  -9.80983  L
H-HC-0.100000         0     1.41364  -2.25882  -12.38917  L
H-HC-0.100000         0     1.84478  -0.54454  -12.18269  L
H-HC-0.100000         0     0.53214  -0.99799  -13.28487  L
N-N--0.347900         0    -3.02187  -0.29003  -8.78091  L
C-CT--0.263700        -1   -3.39004   1.08901  -8.36133  L
C-C-0.734100          0    -2.13662   1.97022  -8.4351   L
O-O--0.589400         0    -1.01665   1.46901  -8.53788  L
C-CT--0.000700        0    -4.05659   1.04283  -6.98151  L
C-CT-0.039000         0    -4.79252   2.34329  -6.63143  L
C-CT-0.048600         0    -5.61687   2.19928  -5.35703  L
N-N2--0.529500        0    -4.77734   2.05938  -4.16224  L
C-CA-0.807600         0    -5.24289   1.91233  -2.94166  L
N-N2--0.862700        0    -6.47416   1.61248  -2.68959  L
N-N2--0.862700        0    -4.48512   2.07105  -1.90737  L
H-H-0.274700          0    -2.67599  -0.91646  -8.06421  L
H-H1-0.156000         0    -4.10428   1.48071  -9.08838  L
H-HC-0.032700         0    -3.31417   0.81418  -6.2183   L
H-HC-0.032700         0    -4.79764   0.24512  -7.00606  L
H-HC-0.028500         0    -5.46825   2.60317  -7.44747  L
H-HC-0.028500         0    -4.08706   3.15859  -6.48746  L
H-H1-0.068700         0    -6.30451   1.35612  -5.45324  L
H-H1-0.068700         0    -6.19069   3.11631  -5.24245  L
H-H-0.345600          0    -3.79984   2.3452   -4.25278  L
H-H-0.447800          0    -6.77556   1.51775  -1.72965  L
H-H-0.447800          0    -7.01321   1.08062  -3.37243  L
H-H-0.447800          0    -4.88065   1.89414  -0.9967   L
H-H-0.447800          0    -3.52029   2.36214  -2.06111  L
N-N--0.415700         0    -2.32974   3.27898  -8.36556  L
C-CT--0.002400        -1   -1.29496   4.25317  -8.04915  L
C-C-0.597300          0    -1.8468    5.1947   -6.98064  L
O-O--0.567900         0    -2.99346   5.62664  -7.06407  L
C-CT--0.034300        0    -0.85321   4.99731  -9.31452  L
C-CA-0.011800         0    -0.11377   4.1189   -10.30836  L
C-CA--0.125600        0     1.25701   3.85093  -10.13033  L
C-CA--0.125600        0    -0.79979   3.53838  -11.39173  L
C-CA--0.170400        0     1.94306   3.03114  -11.04408  L
C-CA--0.170400        0    -0.11752   2.70832  -12.29882  L
C-CA--0.107200        0     1.25615   2.46103  -12.1306  L
H-H-0.271900          0    -3.27628   3.61547  -8.27572  L
H-H1-0.097800         0    -0.42754   3.74364  -7.62841  L
H-HC-0.029500         0    -0.19691   5.81777  -9.02333  L
H-HC-0.029500         0    -1.72788   5.43865  -9.79558  L
H-HA-0.133000         0     1.77792   4.26632  -9.28137  L
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 H-HA-0.133000        0    -1.85931   3.7134   -11.51569  L
 H-HA-0.143000        0     2.99246   2.83614  -10.89936  L
 H-HA-0.143000        0    -0.66169   2.25202  -13.11359  L
 H-HA-0.129700        0     1.77267   1.82202  -12.83018  L
 N-N--0.516300        0    -1.04435   5.464    -5.95688  L
 C-CT-0.038100        0    -1.47104   6.10798  -4.71918  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.75516   7.4617   -4.55932  L
 O-O--0.581900        0    -0.03504   7.70398  -3.58363  L
 C-CT--0.030300       0    -1.21875   5.15467  -3.54134  H
 C-C-0.799400         0    -1.89037   3.78358  -3.58473  H
 O-O2--0.801400       0    -2.10977   3.25902  -2.36918  H
 O-O2--0.801400       0    -2.21921   3.1241   -4.5407   H
 H-H-0.293600         0    -0.16041   4.9697   -5.92872  L
 H-H1-0.088000        0    -2.54244   6.31259  -4.76002  L
 H-HC--0.012200       0    -1.56118   5.6561   -2.63233  H
 H-HC--0.012200       0    -0.14137   4.97236  -3.44639  H
 N-N--0.516300        0    -0.96701   8.33506  -5.54672  L
 C-CT-0.038100        0    -0.31792   9.63498  -5.77991  L
 C-C-0.536600         0    -0.87426   10.78282  -4.91604  L
 O-O--0.581900        0    -0.72341   11.96023  -5.24276  L
 C-CT--0.030300       0    -0.44042   9.97642  -7.28059  L
 C-C-0.799400         0    -1.8534    10.36839  -7.73615  L
 O-O2--0.801400       0    -2.81788   9.75764  -7.2206   L
 O-O2--0.801400       0    -1.94637   11.2154  -8.65351  L
 H-H-0.293600         0    -1.69274   8.12104  -6.22734  L
 H-H1-0.088000        0     0.73929   9.53695  -5.54469  L
 H-HC--0.012200       0    -0.13473   9.11248  -7.86746  L
 H-HC--0.012200       0     0.2498    10.79109  -7.50842  L
 N-N--0.415700        0    -1.48996   10.45233  -3.77763  L
 C-CT--0.038900       -1   -2.23412   11.37313  -2.90065  L
 C-C-0.597300         0    -1.34794   12.54733  -2.35467  L
 O-O--0.567900        0    -1.90523   13.52305  -1.8533   L
 C-CT-0.365400        0    -2.90753   10.63845  -1.75087  L
 O-OH--0.676100       0    -2.04341   9.75138  -1.06641  L
 C-CT--0.243800       -1   -4.02791   9.83157  -2.37769  L
 H-H-0.271900         0    -1.49337   9.46916  -3.5491   L
 H-H1-0.100700        0    -3.00922   11.85332  -3.4976   L
 H-H1-0.004300        0    -3.32879   11.35192  -1.04308  L
 H-HC-0.064200        0    -4.72115   10.49651  -2.89126  L
 H-HC-0.064200        0    -4.54801   9.3156   -1.5774   L
 H-HC-0.064200        0    -3.63919   9.09239  -3.07812  L
 H-HO-0.410200        0    -1.86081   10.18056  -0.19526  L
 N-N--0.415700        0     0.00155   12.53947  -2.495    L
 C-CT-0.014300        -1    0.90865   13.71775  -2.36802  L
 C-C-0.597300         0     1.85805   13.82331  -3.59043  L
 O-O--0.567900        0     3.00339   13.3748  -3.49816  L
 C-CT--0.204100       0     1.64876   13.72232  -1.01884  L
 C-C-0.713000         0     2.4458    15.00895  -0.81814  L
 O-O--0.593100        0     2.69027   15.80843  -1.712    L
 N-N--0.919100        0     2.88454   15.27724   0.38513  L
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 H-H-0.271900         0     0.35138   11.74822  -3.02108  L
 H-H1-0.104800        0     0.2839    14.60946  -2.36056  L
 H-HC-0.079700        0     2.3284    12.87357  -0.97047  L
 H-HC-0.079700        0     0.91544   13.63296  -0.21614  L
 H-H-0.419600         0     3.38125   16.14277   0.46862  L
 H-H-0.419600         0     2.64642   14.69186   1.17428  L
 N-N--0.254800        0     1.45759   14.49131  -4.69729  L
 C-CT--0.026600       -1    2.20648   14.50652  -5.96547  L
 C-C-0.589600         0     3.57565   15.17315  -5.90147  L
 O-O--0.574800        0     4.3985    15.0059  -6.7992   L
 C-CT--0.007000       0     1.27136   15.14111  -6.99952  L
 C-CT-0.018900        0     0.32145   15.98862  -6.15794  L
 C-CT-0.019200        0     0.18887   15.18822  -4.8647   L
 H-H1-0.064100        0     2.37083   13.47093  -6.26248  L
 H-HC-0.025300        0     0.70309   14.35336  -7.4982   L
 H-HC-0.025300        0     1.80759   15.74207  -7.73509  L
 H-HC-0.021300        0    -0.64304   16.12355  -6.64853  L
 H-HC-0.021300        0     0.78414   16.95311  -5.94399  L
 H-H1-0.039100        0    -0.01285   15.86562  -4.03492  L
 H-H1-0.039100        0    -0.61931   14.46228  -4.96129  L
 N-N--0.415700        0     3.87466   15.91853  -4.84014  L
 C-CT--0.025200       -1    5.0423    16.7877  -4.80377  L
 C-C-0.597300         0     6.38765   16.14868  -4.47128  L
 O-O--0.567900        0     7.32137   16.81818  -4.03436  L
 H-H-0.271900         0     3.22528   15.91902  -4.06154  L
 H-H1-0.069800        0     4.86248   17.56168  -4.058    L
 H-H1-0.069800        0     5.14601   17.28576  -5.76828  L
 N-N--0.347900        0     6.4809    14.85254  -4.72531  L
 C-CT--0.240000       -1    7.64312   13.96785  -4.62042  L
 C-C-0.734100         0     7.57301   12.89823  -5.74712  L
 O-O--0.589400        0     8.35731   11.94987  -5.72963  L
 C-CT--0.009400       0     7.64142   13.34038  -3.19311  L
 C-CT-0.018700        0     6.41591   12.4271  -3.05637  L    H-HC
590   0.        0.
 C-CT--0.047900       0     6.04184   11.68031  -1.77496  H
 C-CT--0.014300       0     4.8277    10.88561  -2.26913  H
 N-N3--0.385400       0     4.17426   9.98062  -1.31382  H
 H-H-0.274700         0     5.60769   14.45827  -5.0558   L
 H-H1-0.142600        0     8.55733   14.54514  -4.75985  L
 H-HC-0.036200        0     7.5992    14.12933  -2.44032  L
 H-HC-0.036200        0     8.54968   12.75556  -3.04329  L
 H-HC-0.010300        0     6.57249   11.65258  -3.78983  L
 H-HC-0.010300        0     5.54092   13.0135  -3.32553  L
 H-HC-0.062100        0     5.7781    12.39361  -0.99277  H
 H-HC-0.062100        0     6.8571    11.03515  -1.44893  H
 H-HP-0.113500        0     5.1268    10.24701  -3.10739  H
 H-HP-0.113500        0     4.07933   11.57931  -2.67596  H
 H-H-0.340000         0     3.31609   9.67787  -1.78372  H
 H-H-0.340000         0     3.88537   10.50361  -0.4815   H
 H-H-0.340000         0     5.09101   8.78921  -0.76486  H
 N-N--0.516300        0     6.60488   12.98572  -6.67358  L
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C-CT-0.039700        -1    6.09044   11.88023  -7.51092  L
C-C-0.536600         0     6.27461   12.19781  -9.02349  L
O-O--0.581900        0     6.07397   13.33107  -9.45226  L
C-CT-0.056000        0     4.64094   11.51623  -7.11395  L
C-CT-0.013600        0     4.64002   11.17335  -5.61563  L
C-C-0.805400         0     3.66682   10.13129  -5.05357  L
O-O2--0.818800       0     2.65752   10.50245  -4.42316  L
O-O2--0.818800       0     4.11077   8.96413  -4.98233  L
H-H-0.293600         0     6.05206   13.83451  -6.73311  L
H-H1-0.110500        0     6.69819   10.99591  -7.31907  L
H-HC--0.017300       0     4.31776   10.67363  -7.70823  L
H-HC--0.017300       0     3.97124   12.3506  -7.31182  L
H-HC--0.042500       0     4.53446   12.10663  -5.07025  L
H-HC--0.042500       0     5.62519   10.76668  -5.39913  L
N-N--0.415700        0     6.73931   11.22577  -9.83577  L
C-CT--0.149000       -1    7.12859   11.40979  -11.25216  L
H-H-0.271900         0     6.86409   10.31366  -9.42503  L
H-H1-0.097600        0     7.90984   12.16868  -11.3206  L
H-H1-0.097600        0     6.26238   11.7514  -11.8226  L
H-H1-0.097600        0     7.49083   10.47036  -11.67049  L
C-CT--0.366200       0     10.00278   2.31482  -12.00926  L
C-C-0.597200         0     8.99909   1.46136  -11.27173  L
O-O--0.567900        0     9.29859   0.97278  -10.18795  L
H-HC-0.112300        0     10.5677   2.88911  -11.27688  L
H-HC-0.112300        0     9.50007   2.9979   -12.69058  L
H-HC-0.112300        0     10.67927   1.66036  -12.55507  L
N-N--0.415700        0     7.80896   1.29791  -11.85618  L
C-CT--0.059700       -1    6.71761   0.47636  -11.30652  L
C-C-0.597300         0     6.06556  -0.3753   -12.41353  L
O-O--0.567900        0     6.49025  -1.50557  -12.63159  L
C-CT-0.130300        0     5.7001    1.32104  -10.48118  L
C-CT--0.043000       0     6.38626   2.14868  -9.36423  L
C-CT--0.320400       0     4.61746   0.41681  -9.85107  L
C-CT--0.066000       0     5.44102   3.05364  -8.5627   L
H-H-0.271900         0     7.6856    1.72516  -12.75891  L
H-H1-0.086900        0     7.16723  -0.23745  -10.61911  L
H-HC-0.018700        0     5.2118    2.02211  -11.15908  L
H-HC-0.023600        0     7.12974   2.8063   -9.81268  L
H-HC-0.023600        0     6.90026   1.47685  -8.6747   L
H-HC-0.088200        0     4.16214  -0.24276  -10.58835  L
H-HC-0.088200        0     3.81575   1.02343  -9.42992  L
H-HC-0.088200        0     5.04896  -0.19017  -9.05604  L
H-HC-0.018600        0     4.77967   2.45771  -7.93509  L
H-HC-0.018600        0     4.84859   3.66765  -9.24146  L
H-HC-0.018600        0     6.03149   3.70646  -7.91935  L
N-N--0.415700        0     5.04906   0.14668  -13.11744  L
C-CT--0.149000       -1    4.27819  -0.58582  -14.1253  L
H-H-0.271900         0     4.74983   1.07639  -12.86933  L
H-H1-0.097600        0     3.8717   -1.49925  -13.68556  L
H-H1-0.097600        0     4.92672  -0.86108  -14.95895  L
H-H1-0.097600        0     3.45499   0.02823  -14.49393  L
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C-CT--0.366200       -1   -5.10038   16.94463  -3.11783  L
C-C-0.597200         0    -5.67247   16.1742  -1.94105  L
O-O--0.567900        0    -5.5192    16.62299  -0.80799  L
H-HC-0.112300        0    -5.90985   17.34333  -3.72415  L
H-HC-0.112300        0    -4.46958   16.27969  -3.70679  L
H-HC-0.112300        0    -4.4915    17.76204  -2.73598  L
N-N--0.254800        0    -6.39191   15.06718  -2.18725  L
C-CT--0.026600       -1   -7.07801   14.31316  -1.14441  L
C-C-0.589600         0    -6.2213    13.20947  -0.52522  L
O-O--0.574800        0    -5.69599   12.32562  -1.19978  L
C-CT--0.007000       0    -8.28342   13.70604  -1.87221  L
C-CT-0.018900        0    -7.7496    13.42518  -3.2799   L
C-CT-0.019200        0    -6.75347   14.56343  -3.50848  L
H-H1-0.064100        0    -7.43517   14.98435  -0.36275  L
H-HC-0.025300        0    -9.08189   14.44723  -1.92973  L
H-HC-0.025300        0    -8.64781   12.8     -1.38803  L
H-HC-0.021300        0    -8.54875   13.4356  -4.02142  L
H-HC-0.021300        0    -7.2277    12.46826  -3.30444  L
H-H1-0.039100        0    -5.87434   14.19147  -4.03733  L
H-H1-0.039100        0    -7.23437   15.35362  -4.08577  L
N-N--0.415700        0    -6.1548    13.25088   0.79775  L
C-CT--0.023700       -1   -5.29954   12.41651   1.62889  L
C-C-0.597300         0    -5.48687   10.89006   1.50336  L
O-O--0.567900        0    -6.58356   10.40584   1.20985  L
C-CT-0.034200        0    -5.5476    12.78797   3.10468  L
C-CT-0.001800        0    -5.11263   14.20906   3.49333  L
S-S--0.273700        0    -3.32912   14.47421   3.70275  L
C-CT--0.053600       -1   -3.02098   13.50784   5.20974  L
H-H-0.271900         0    -6.62641   14.01916   1.24173  L
H-H1-0.088000        0    -4.25802   12.63804   1.38336  L
H-HC-0.024100        0    -5.02962   12.07936   3.75091  L
H-HC-0.024100        0    -6.61483   12.68717   3.30908  L
H-H1-0.044000        0    -5.59409   14.46103   4.43832  L
H-H1-0.044000        0    -5.47743   14.91229   2.74483  L
H-H1-0.068400        0    -3.20796   12.45113   5.01724  L
H-H1-0.068400        0    -3.66867   13.85325   6.0146   L
H-H1-0.068400        0    -1.97883   13.62018   5.5073   L
N-N--0.415700        0    -4.4215    10.14245   1.8288   L
C-CT--0.001400       -1   -4.2905    8.68934   1.68581  L
C-C-0.597300         0    -5.53808   7.82419   1.98648  L
O-O--0.567900        0    -6.12176   7.31551   1.03461  L
C-CT--0.015200       0    -3.0288    8.1439    2.37575  L
C-CA--0.001100       0    -2.9758    6.63802   2.58622  L
C-CA--0.190600       0    -3.32135   5.73912   1.55712  L
C-CA--0.190600       0    -2.66294   6.14086   3.8611   L
C-CA--0.234100       0    -3.36239   4.35294   1.81755  L
C-CA--0.234100       0    -2.75997   4.76742   4.13649  L
C-C-0.322600         0    -3.1112    3.86767   3.11631  L
O-OH--0.557900       0    -3.22872   2.54085   3.37491  L
H-H-0.271900         0    -3.54628   10.63407   1.9935   L
H-H1-0.087600        0    -4.11528   8.53317   0.62147  L
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H-HC-0.029500        0    -2.93632   8.63392   3.34453  L
H-HC-0.029500        0    -2.16618   8.404     1.76949  L
H-HA-0.169900        0    -3.61821   6.12643   0.58969  L
H-HA-0.169900        0    -2.4258    6.82741   4.66015  L
H-HA-0.165600        0    -3.66266   3.64484   1.06151  L
H-HA-0.165600        0    -2.63292   4.41783   5.14781  L
H-HO-0.399200        0    -3.53765   2.40914   4.29291  L
N-N--0.516300        0    -5.89512   7.52805   3.2445   L
C-CT-0.038100       -1    -6.83221   6.43743   3.61715  L
C-C-0.536600         0    -8.23858   6.63826   3.05036  L
O-O--0.581900        0    -8.88672   5.66878   2.66459  L
C-CT--0.030300       0    -6.89546   6.27212   5.14747  L
C-C-0.799400         0    -5.61918   5.65738   5.73539  L
O-O2--0.801400       0    -5.48914   4.41006   5.66976  L
O-O2--0.801400       0    -4.77153   6.42997   6.24755  L
H-H-0.293600         0    -5.4022    8.0127    3.99044  L
H-H1-0.088000        0    -6.44692   5.5023    3.21652  L
H-HC--0.012200       0    -7.72847   5.61214   5.39257  L
H-HC--0.012200       0    -7.10039   7.2369    5.61377  L
N-N--0.415700        0    -8.6954    7.89017   2.96302  L
C-CT--0.002400       0    -9.89041   8.27283   2.20994  L
C-C-0.597300         0    -9.78343   7.83229   0.74193  L
O-O--0.567900        0    -10.62685   7.08343   0.2487   L
C-CT--0.034300       0    -10.10964   9.7887    2.33188  L
C-CA-0.011800        0    -11.16507   10.32494   1.38233  L
C-CA--0.125600       0    -12.53152   10.127    1.65577  L
C-CA--0.125600       0    -10.77718   10.96307   0.18819  L
C-CA--0.170400       0    -13.50499   10.56936   0.74149  L
C-CA--0.170400       0    -11.74964   11.40287  -0.72662  L
C-CA--0.107200       0    -13.11414   11.20668  -0.44984  L
H-H-0.271900         0    -8.05348   8.60884   3.2666   L
H-H1-0.097800        0    -10.7545   7.76165   2.63566  L
H-HC-0.029500        0    -9.16858   10.30396   2.13278  L
H-HC-0.029500        0    -10.40039   10.02232   3.35679  L
H-HA-0.133000        0    -12.8331   9.61574   2.55875  L
H-HA-0.133000        0    -9.72766   11.08887  -0.04366  L
H-HA-0.143000        0    -14.55245   10.40284   0.94725  L
H-HA-0.143000        0    -11.44145   11.87245  -1.65009  L
H-HA-0.129700        0    -13.86053   11.53261  -1.16     L
N-N--0.415700        0    -8.7508    8.28815   0.03556  L
C-CT--0.038900      -1    -8.55781   7.99933  -1.38969  L
C-C-0.597300         0    -8.37729   6.52209  -1.6923   L
O-O--0.567900        0    -9.01727   5.97392  -2.58633  L
C-CT-0.365400        0    -7.41149   8.84371  -1.95833  L
O-OH--0.676100       0    -7.67548   10.20735  -1.70305  L
C-CT--0.243800       0    -7.27235   8.69772  -3.47407  L
H-H-0.271900         0    -8.08233   8.90763   0.48361  L
H-H1-0.100700        0    -9.46363   8.31062  -1.90962  L
H-H1-0.004300        0    -6.48737   8.54992  -1.46705  L
H-HC-0.064200        0    -8.22411   8.92004  -3.95681  L
H-HC-0.064200        0    -6.96477   7.6842   -3.73048  L
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H-HC-0.064200        0    -6.5212    9.39095  -3.84968  L
H-HO-0.410200        0    -6.8304    10.66539  -1.56737  L
N-N--0.415700        0    -7.5371    5.87207  -0.89904  L
C-CT--0.058100       -1   -7.39444   4.42977  -0.76968  L
C-C-0.597300         0    -8.73907   3.72906  -0.63563  L
O-O--0.567900        0    -9.04734   2.86927  -1.46054  L
C-CT--0.007400       0    -6.46138   4.2031    0.41887  L
C-CC-0.186800        0    -6.38452   2.80316   0.94472  L
N-NB--0.543200       0    -6.47156   1.64956   0.17731  L
C-CW--0.220700       0    -6.26045   2.46352   2.25594  L
C-CR-0.163500        0    -6.44463   0.62548   1.03481  L
N-NA--0.279500       0    -6.29824   1.09047   2.28521  L
H-H-0.271900         0    -7.08417   6.4489   -0.19676  L
H-H1-0.136000        0    -6.92525   4.03703  -1.67082  L
H-HC-0.036700        0    -6.79573   4.82836   1.2393   L
H-HC-0.036700        0    -5.46912   4.53003   0.1216   L
H-H4-0.186200        0    -6.18257   3.13638   3.10221  L
H-H-0.333900         0    -6.27505   0.49586   3.11175  L
H-H5-0.143500        0    -6.54759  -0.41568   0.7534   L
N-N--0.415700        0    -9.54227   4.10213   0.36629  L
C-CT-0.021300        -1   -10.83751   3.4727    0.57534  L
C-C-0.597300         0    -11.75169   3.51904  -0.62707  L
O-O--0.567900        0    -12.36016   2.51584  -0.99669  L
C-CT--0.123100       0    -11.49456   3.86149   1.91766  L
S-SH--0.311900       0    -12.59665   5.30288   1.84268  L
H-H-0.271900         0    -9.23968   4.82158   1.01504  L
H-H1-0.112400        0    -10.61306   2.40993   0.6779   L
H-H1-0.111200        0    -10.72366   4.03397   2.66777  L
H-H1-0.111200        0    -12.08847   3.0122    2.25909  L
H-HS-0.193300        0    -11.69752   6.15022   1.3237   L
N-N--0.415700        0    -11.79872   4.68326  -1.25278  L
C-CT--0.059700       -1   -12.61492   4.90648  -2.41805  L
C-C-0.597300         0    -12.11745   4.20192  -3.68116  L
O-O--0.567900        0    -12.92642   3.57547  -4.36433  L
C-CT-0.130300        0    -12.8479   6.43167  -2.59348  L
C-CT--0.043000       0    -14.18417   6.87179  -1.94503  L
C-CT--0.320400       -1   -12.75739   6.94063  -4.03777  L
C-CT--0.066000       -1   -15.47297   6.46731  -2.69166  L
H-H-0.271900         0    -11.25956   5.44733  -0.85894  L
H-H1-0.086900        0    -13.58383   4.45151  -2.21502  L
H-HC-0.018700        0    -12.05555   6.95611  -2.05559  L
H-HC-0.023600        0    -14.17793   7.95885  -1.85342  L
H-HC-0.023600        0    -14.22781   6.46562  -0.93324  L
H-HC-0.088200        0    -11.73742   6.83498  -4.4091   L
H-HC-0.088200        0    -13.01321   7.99977  -4.07033  L
H-HC-0.088200        0    -13.43764   6.38869  -4.68793  L
H-HC-0.018600        0    -16.33825   6.77203  -2.10278  L
H-HC-0.018600        0    -15.50832   5.38745  -2.83492  L
H-HC-0.018600        0    -15.5211   6.96295  -3.66107  L
N-N--0.415700        0    -10.82523   4.29661  -4.01175  L
C-CT--0.024900       -1   -10.25228   3.57055  -5.15061  L
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C-C-0.597300          0    -10.51393   2.05867  -4.98275  L
O-O--0.567900         0    -10.92257   1.42345  -5.9473   L
C-CT-0.211700         0    -8.76384    3.841    -5.30276  L
O-OH--0.654600        0    -8.31942    3.27972  -6.52491  L
H-H-0.271900          0    -10.21658    4.84004  -3.40741  L
H-H1-0.084300         0    -10.75693    3.90088  -6.05923  L
H-H1-0.035200         0    -8.22802    3.39766  -4.46226  L
H-H1-0.035200         0    -8.58256    4.91684  -5.31472  L
H-HO-0.427500         0    -8.87988    2.52637  -6.75937  L
N-N--0.516300         0    -10.30992    1.48047  -3.78729  L
C-CT-0.038100         -1   -10.55508    0.05004  -3.50835  L
C-C-0.536600          0    -12.03281  -0.35798  -3.61626  L
O-O--0.581900         0    -12.36288  -1.31504  -4.32192  L
C-CT--0.030300        0    -9.94      -0.37368  -2.16333  L
C-C-0.799400          0    -8.46496   -0.75269  -2.30843  L
O-O2--0.801400        0    -7.87865   -0.52777  -3.39136  L
O-O2--0.801400        0    -7.87812   -1.28494  -1.33927  L
H-H-0.293600          0    -9.96482    2.05733  -3.02658  L
H-H1-0.088000         0    -10.06387  -0.51633  -4.29822  L
H-HC--0.012200        0    -10.47269  -1.24578  -1.7836   L
H-HC--0.012200        0    -10.05462    0.42345  -1.4282   L
N-N--0.415700         0    -12.92447    0.3688   -2.93847  L
C-CT-0.033700         -1   -14.3781    0.23852  -3.06064  L
C-C-0.597300          0    -14.84915    0.25398  -4.52656  L
O-O--0.567900         0    -15.67055  -0.56931  -4.92576  L
C-CT--0.182500        -1   -14.99195    1.39605  -2.33271  L
H-H-0.271900          0    -12.57108    1.13351  -2.37199  L
H-H1-0.082300         0    -14.70098  -0.69914  -2.60743  L
H-HC-0.060300         0    -14.72721    1.34891  -1.27591  L
H-HC-0.060300         0    -16.07836    1.34483  -2.41656  L
H-HC-0.060300         0    -14.64806    2.34378  -2.74625  L
N-N--0.415700         0    -14.36234    1.23108  -5.29836  L
C-CT--0.025200        -1   -14.7364    1.48143  -6.68662  L
C-C-0.597300          0    -14.24435    0.42165  -7.6686   L
O-O--0.567900         0    -14.98534    0.01532  -8.5585   L
H-H-0.271900          0    -13.70481    1.87392  -4.8684   L
H-H1-0.069800         0    -14.3278    2.4427   -6.99571  L
H-H1-0.069800         0    -15.82276    1.5288   -6.75968  L
N-N--0.516300         0    -12.99114    0.00068  -7.51488  L
C-CT-0.039700         -1   -12.35403  -1.0871   -8.26201  L
C-C-0.536600          0    -13.08162  -2.43399  -8.09018  L
O-O--0.581900         0    -13.2146   -3.19306  -9.04681  L
C-CT-0.056000         0    -10.89018  -1.14231  -7.79762  L
C-CT-0.013600         0    -10.01078  -2.22928  -8.42479  L
C-C-0.805400          0    -9.57911   -1.93672  -9.86376  L
O-O2--0.818800        0    -9.57046   -2.8794   -10.6866  L
O-O2--0.818800        0    -9.09888   -0.81246  -10.12397  L
H-H-0.293600          0    -12.42986    0.44411  -6.79426  L
H-H1-0.110500         0    -12.36873  -0.84877  -9.3265   L
H-HC--0.017300        0    -10.89998  -1.29897  -6.72213  L
H-HC--0.017300        0    -10.42428  -0.17294  -7.97577  L
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H-HC--0.042500       0    -10.53211  -3.18092  -8.365    L
H-HC--0.042500       0    -9.10304  -2.31659  -7.82484  L
N-N--0.415700        0    -13.53903  -2.7402   -6.87106  L
C-CT--0.025200       -1   -14.23755  -3.9875   -6.52475  L
C-C-0.597300         0    -13.48832  -4.84736  -5.52265  L
O-O--0.567900        0    -13.82925  -6.02225  -5.36594  L
H-H-0.271900         0    -13.42255  -2.02716  -6.16036  L
H-H1-0.069800        0    -14.40809  -4.58582  -7.42019  L
H-H1-0.069800        0    -15.20691  -3.73672  -6.09589  L
N-N--0.415700        0    -12.47894  -4.28718  -4.839    L
C-CT--0.059700       -1   -11.74578  -4.99381  -3.78792  L
C-C-0.597300         0    -12.76629  -5.54247  -2.78562  L
O-O--0.567900        0    -13.69746  -4.84593  -2.38704  L
C-CT-0.130300        0    -10.6863  -4.09631  -3.0942   L
C-CT--0.043000       0    -9.36213  -4.02113  -3.87439  L
C-CT--0.320400       0    -10.26603  -4.60107  -1.6962   L
C-CT--0.066000       0    -9.44349  -3.45275  -5.28414  L
H-H-0.271900         0    -12.32559  -3.2924   -4.96524  L
H-H1-0.086900        0    -11.23981  -5.83259  -4.24775  L
H-HC-0.018700        0    -11.0962  -3.09654  -2.97432  L
H-HC-0.023600        0    -8.94677  -5.01832  -3.93736  L
H-HC-0.023600        0    -8.66535  -3.402    -3.31249  L
H-HC-0.088200        0    -9.51863  -3.92992  -1.2686   L
H-HC-0.088200        0    -9.84934  -5.60687  -1.76349  L
H-HC-0.088200        0    -11.11557  -4.60229  -1.0218   L
H-HC-0.018600        0    -8.44377  -3.40575  -5.71334  L
H-HC-0.018600        0    -9.85511  -2.45126  -5.23549  L
H-HC-0.018600        0    -10.06605  -4.08296  -5.91525  L
N-N--0.415700        0    -12.57996  -6.79477  -2.36658  L
C-CT--0.025200       -1   -13.43396  -7.44061  -1.36179  L
C-C-0.597300         0    -12.882   -7.37764   0.04544  L
O-O--0.567900        0    -13.6106  -7.17829   1.01536  L
H-H-0.271900         0    -11.8344  -7.29949  -2.82884  L
H-H1-0.069800        0    -13.56416  -8.48812  -1.62892  L
H-H1-0.069800        0    -14.42131  -6.97617  -1.36044  L
N-N--0.415700        0    -11.57345  -7.5682    0.13902  L
C-CT--0.058100       -1   -10.82117  -7.56008   1.37519  L
C-C-0.597300         0    -9.44501  -6.91388   1.10852  L
O-O--0.567900        0    -8.70809  -7.39535   0.24897  L
C-CT--0.007400       0    -10.66973  -9.00439   1.88333  L
C-CC-0.186800        0    -11.96591  -9.59605   2.38908  L
N-NB--0.543200       0    -12.56932  -9.31748   3.61874  L
C-CW--0.220700       0    -12.7782  -10.42886   1.67651  L
C-CR-0.163500        0    -13.73723  -9.97465   3.61169  L
N-NA--0.279500       0    -13.88857  -10.65492   2.46136  L
H-H-0.271900         0    -11.05149  -7.68462  -0.71779  L
H-H1-0.136000        0    -11.34282  -6.9746    2.13396  L
H-HC-0.036700        0    -9.93394  -9.03009   2.68463  L
H-HC-0.036700        0    -10.2833  -9.63047   1.0776   L
H-H4-0.186200        0    -12.59004  -10.78917   0.67535  L
H-H-0.333900         0    -14.70316  -11.19457   2.20919  L
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H-H5-0.143500        0    -14.45902  -9.94737   4.41787  L
N-N--0.415700        0    -9.09818   -5.81144   1.78523  L
C-CT--0.024900       -1   -7.83928   -5.07447   1.5548   L
C-C-0.597300         0    -6.64624   -5.70259   2.27646  L
O-O--0.567900        0    -6.68908   -5.97817   3.47512  L
C-CT-0.211700        0    -7.97149   -3.58248   1.88785  L
O-OH--0.654600       0    -6.69691   -2.95098   1.861    L
H-H-0.271900         0    -9.71284   -5.5206    2.53764  L
H-H1-0.084300        0    -7.62659   -5.11892   0.48596  L
H-H1-0.035200        0    -8.41827   -3.47095   2.86905  L
H-H1-0.035200        0    -8.62733   -3.10545   1.15719  L
H-HO-0.427500        0    -6.71913   -2.18635   2.46654  L
N-N--0.415700        0    -5.55312   -5.89578   1.53614  L
C-CT--0.051800       -1   -4.25124   -6.29608   2.06521  L
C-C-0.597300         0    -3.36917   -5.08073   2.2889   L
O-O--0.567900        0    -3.16259   -4.29412   1.36584  L
C-CT--0.110200       0    -3.56851   -7.27901   1.08974  L
C-CT-0.353100        0    -4.07672   -8.73363   1.11492  L
C-CT--0.412100       0    -5.46439   -8.91202   0.49795  L
C-CT--0.412100       0    -3.10511   -9.61204   0.31988  L
H-H-0.271900         0    -5.63055   -5.68197   0.55367  L
H-H1-0.092200        0    -4.38576   -6.80071   3.02518  L
H-HC-0.045700        0    -2.51271   -7.3086    1.34927  L
H-HC-0.045700        0    -3.63682   -6.89291   0.07542  L
H-HC--0.036100       0    -4.09499   -9.08932   2.14537  L
H-HC-0.100000        0    -5.48796   -8.49848  -0.51092  L
H-HC-0.100000        0    -6.21528   -8.41396   1.10898  L
H-HC-0.100000        0    -5.72161   -9.96941   0.458    L
H-HC-0.100000        0    -2.10708   -9.54602   0.75233  L
H-HC-0.100000        0    -3.07322   -9.28343  -0.71958  L
H-HC-0.100000        0    -3.43474   -10.65018   0.35524  L
N-N--0.415700        0    -2.81243   -4.96718   3.48704  L
C-CT-0.021300        -1   -1.88722   -3.89956   3.83526  L
C-C-0.597300         0    -0.74835   -4.41082   4.73508  L
O-O--0.567900        0    -0.75131   -5.57136   5.14931  L
C-CT--0.123100       0    -2.71647   -2.78847   4.48755  L
S-SH--0.311900       0    -1.81221   -1.22128   4.49645  L
H-H-0.271900         0    -3.05936   -5.63564   4.20889  L
H-H1-0.112400        0    -1.4292    -3.49673   2.92831  L
H-H1-0.111200        0    -2.98954   -3.07078   5.50608  L
H-H1-0.111200        0    -3.62793   -2.64192   3.90749  L
H-HS-0.193300        0    -2.71756   -0.54045   5.21374  L
N-N--0.415700        0     0.23588   -3.57285   5.06102  L
C-CT--0.038900       -1    1.34483   -3.94749   5.9527   L
C-C-0.597300         0     1.46615   -3.05494   7.16416  L
O-O--0.567900        0     0.79465   -2.04032   7.32553  L
C-CT-0.365400        0     2.70028   -4.06779   5.22597  L
O-OH--0.676100       0     3.13565   -2.8559    4.64686  L
C-CT--0.243800       0     2.67517   -5.15579   4.15604  L
H-H-0.271900         0     0.15374   -2.61482   4.74057  L
H-H1-0.100700        0     1.13707   -4.93761   6.35813  L
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H-H1-0.004300        0     3.45707  -4.37099   5.94966  L
H-HC-0.064200        0     1.98605  -4.89173   3.35499  L
H-HC-0.064200        0     2.35362  -6.09928   4.5985   L
H-HC-0.064200        0     3.67377  -5.27835   3.74677  L
H-HO-0.410200        0     3.48436  -2.27636   5.3635   L
N-N--0.415700        0     2.31076  -3.53344   8.06849  L
C-CT--0.051800       -1    2.22261  -3.2387    9.47635  L
C-C-0.597300         0     2.30144  -1.74015   9.85824  L
O-O--0.567900        0     1.7374   -1.35429   10.8726  L
C-CT--0.110200       0     3.23212  -4.10424   10.19894  L
C-CT-0.353100        0     2.93043  -4.18621   11.69688  L
C-CT--0.412100       0     1.59275  -4.84301   12.04966  L
C-CT--0.412100       -1    4.02844  -5.07554   12.21806  L
H-H-0.271900         0     2.77778  -4.38627   7.81728  L
H-H1-0.092200        0     1.22215  -3.5528    9.77501  L
H-HC-0.045700        0     4.22681  -3.68468   10.03966  L
H-HC-0.045700        0     3.19918  -5.11219   9.78023  L
H-HC--0.036100       0     3.0125   -3.21004   12.17149  L
H-HC-0.100000        0     1.47999  -5.79787   11.53765  L
H-HC-0.100000        0     0.76881  -4.18649   11.7771  L
H-HC-0.100000        0     1.5298   -4.99779   13.12776  L
H-HC-0.100000        0     3.9203   -5.16945   13.29943  L
H-HC-0.100000        0     5.00336  -4.63213   12.01781  L
H-HC-0.100000        0     3.96738  -6.06981   11.77573  L
N-N--0.516300        0     2.96918  -0.89099   9.07269  L
C-CT-0.039700        -1    3.09426   0.56287   9.31789  L
C-C-0.536600         0     1.84439   1.4114    8.98697  L
O-O--0.581900        0     1.91979   2.64232   8.95638  L
C-CT-0.056000        0     4.34687   1.07833   8.57195  L
C-CT-0.013600        0     4.33479   0.94986   7.03419  L
C-C-0.805400         0     4.95932  -0.35225   6.51911  L
O-O2--0.818800       0     4.32124  -1.43139   6.57417  L
O-O2--0.818800       0     6.14194  -0.33559   6.08817  L
H-H-0.293600         0     3.31451  -1.25528   8.18914  L
H-H1-0.110500        0     3.26424   0.71527   10.38474  L
H-HC--0.017300       0     5.22683   0.56159   8.95922  L
H-HC--0.017300       0     4.47625   2.13252   8.81981  L
H-HC--0.042500       0     4.9332    1.76932   6.63489  L
H-HC--0.042500       0     3.31999   1.05929   6.65261  L
N-N--0.415700        0     0.69955   0.75929   8.77508  L
C-CT--0.002400       -1   -0.61735   1.36822   8.55449  L
C-C-0.597300         0    -1.75254   0.72488   9.36646  L
O-O--0.567900        0    -2.93099   1.034     9.17579  L
C-CT--0.034300       0    -0.9761    1.18268   7.07044  L
C-CA-0.011800        0    -0.04987   1.75586   6.01491  L
C-CA--0.125600       0    -0.18002   3.10377   5.64294  L
C-CA--0.125600       0     0.81785   0.91528   5.29051  L
C-CA--0.170400       0     0.49426   3.59229   4.51242  L
C-CA--0.170400       0     1.52968   1.41474   4.18477  L
C-CA--0.107200       0     1.35344   2.75047   3.78485  L
H-H-0.271900         0     0.76426  -0.24789   8.70925  L
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H-H1-0.097800        0    -0.58416   2.43207   8.78865  L
H-HC-0.029500        0    -1.957     1.62364   6.89735  L
H-HC-0.029500        0    -1.08082   0.11283   6.89024  L
H-HA-0.133000        0    -0.83675   3.75343   6.20227  L
H-HA-0.133000        0     0.90726  -0.12622   5.56101  L
H-HA-0.143000        0     0.33365   4.61612   4.2087   L
H-HA-0.143000        0     2.1767    0.76217   3.61664  L
H-HA-0.129700        0     1.87204   3.12486   2.913    L
N-N--0.415700        0    -1.38808  -0.18718   10.25741  L
C-CT--0.003100      -1    -2.24656  -1.07137   11.02774  L
C-C-0.597300         0    -3.49372  -0.38032   11.63809  L
O-O--0.567900        0    -4.6324   -0.72729   11.34061  L
C-CT--0.003600       0    -1.32518  -1.66056   12.11636  L
C-CT--0.064500       0    -1.98066  -2.40785   13.29071  L
C-C-0.695100         0    -1.05225  -2.4427    14.50367  L
O-O--0.608600        0    -0.59387  -3.48786   14.93663  L
N-N--0.940700        0    -0.73888  -1.31643   15.11329  L
H-H-0.271900         0    -0.39112  -0.25846   10.42021  L
H-H1-0.085000        0    -2.61665  -1.87092   10.40038  L
H-HC-0.017100        0    -0.74611  -0.83433   12.53207  L
H-HC-0.017100        0    -0.61613  -2.33498   11.63848  L
H-HC-0.035200        0    -2.22008  -3.42528   12.98044  L
H-HC-0.035200        0    -2.90261  -1.92535   13.60711  L
H-H-0.425100         0    -0.10418  -1.42931   15.87713  L
H-H-0.425100         0    -1.00868  -0.38588   14.78302  L
N-N--0.516300        0    -3.2815    0.54077   12.57189  L
C-CT-0.038100       -1    -4.25872   1.40548   13.27103  L
C-C-0.536600         0    -4.8381    2.47594   12.34358  L
O-O--0.581900        0    -6.03254   2.76717   12.40071  L
C-CT--0.030300       0    -3.53817   2.046     14.4755  L
C-C-0.799400         0    -2.07625   2.35862   14.13751  L
O-O2--0.801400       0    -1.82772   3.36385   13.43653  L
O-O2--0.801400       0    -1.23282   1.45377   14.35768  L
H-H-0.293600         0    -2.30296   0.70069   12.78771  L
H-H1-0.088000        0    -5.09209   0.80406   13.63502  L
H-HC--0.012200       0    -3.5613    1.34027   15.3079  L
H-HC--0.012200       0    -4.05859   2.95315   14.7873  L
N-N--0.415700        0    -3.99403   3.03142   11.46968  L
C-CT-0.014300       -1    -4.34964   4.04524   10.48071  L
C-C-0.597300         0    -5.59645   3.70276   9.66616  L
O-O--0.567900        0    -6.39301   4.58209   9.33921  L
C-CT--0.204100       0    -3.14584   4.3676    9.57514  L
C-C-0.713000         0    -2.17034   5.38294   10.14376  L
O-O--0.593100        0    -1.78483   6.32113   9.46767  L
N-N--0.919100        0    -1.69511   5.25225   11.361   L
H-H-0.271900         0    -3.03054   2.73889   11.54644  L
H-H1-0.104800        0    -4.61016   4.95852   11.01923  L
H-HC-0.079700        0    -3.52549   4.79114   8.64285  L
H-HC-0.079700        0    -2.59984   3.46855   9.32062  L
H-H-0.419600         0    -1.06723   5.98872   11.61617  L
H-H-0.419600         0    -1.93685   4.51912   12.03103  L
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N-N--0.347900        0    -5.78434   2.41438   9.37614  L
C-CT--0.263700       -1   -6.92848   1.90789   8.62632  L
C-C-0.734100         0    -8.32628   2.21383   9.18219  L
O-O--0.589400        0    -9.31262   2.00332   8.47862  L
C-CT--0.000700       0    -6.74336   0.40646   8.34239  L
C-CT-0.039000        0    -7.33014  -0.48331   9.4426   L
C-CT-0.048600        0    -6.91658  -1.94316   9.2742   L
N-N2--0.529500       0    -7.58976  -2.74894   10.29905  L
C-CA-0.807600        0    -7.08115  -3.1299    11.44556  L
N-N2--0.862700       0    -5.80932  -3.21687   11.67518  L
N-N2--0.862700       0    -7.86921  -3.37882   12.4418  L
H-H-0.274700         0    -5.05369   1.77651   9.67377  L
H-H1-0.156000        0    -6.9004    2.41511   7.65976  L
H-HC-0.032700        0    -5.67959   0.18951   8.23011  L
H-HC-0.032700        0    -7.24357   0.16328   7.40346  L
H-HC-0.028500        0    -8.41922  -0.42866   9.41167  L
H-HC-0.028500        0    -6.99231  -0.12714   10.41621  L
H-H1-0.068700        0    -5.83459  -2.00725   9.36667  L
H-H1-0.068700        0    -7.19995  -2.30233   8.288    L
H-H-0.345600         0    -8.59818  -2.81483   10.24587  L
H-H-0.447800         0    -5.44127  -2.27624   11.76469  L
H-H-0.447800         0    -5.32605  -3.57524   10.84164  L
H-H-0.447800         0    -7.44003  -3.61562   13.31103  L
H-H-0.447800         0    -8.84483  -3.10167   12.34091  L
N-N--0.415700        0    -8.44679   2.67596   10.42314  L
C-CT--0.149000       -1   -9.73375   3.00937   11.00741  L
H-H-0.271900         0    -7.59357   2.81348   10.95428  L
H-H1-0.097600        0    -10.31643   3.62015   10.31676  L
H-H1-0.097600        0    -9.58199   3.56115   11.93572  L
H-H1-0.097600        0    -10.28126   2.08958   11.22318  L
C-CT--0.366200       -1   -9.95039   6.22226   8.8173   L
C-C-0.597200         0    -10.66408   5.47909   7.71264  L
O-O--0.567900        0    -11.84692   5.72015   7.51105  L
H-HC-0.112300        0    -9.13337   5.61796   9.21219  L
H-HC-0.112300        0    -10.65874   6.44779   9.6114   L
H-HC-0.112300        0    -9.54949   7.14877   8.41031  L
N-N--0.415700        0    -9.97019   4.56704   7.02818  L
C-CT--0.001400       -1   -10.49194   3.72247   5.93333  L
C-C-0.597300         0    -11.82216   3.01692   6.23539  L
O-O--0.567900        0    -12.69582   2.87514   5.37675  L
C-CT--0.015200       0    -9.35292   2.8294    5.38853  L
C-CA--0.001100       0    -9.73992   1.59652   4.59229  L
C-CA--0.190600       0    -10.34386   0.50459   5.24468  L
C-CA--0.190600       0    -9.42914   1.50679   3.22085  L
C-CA--0.234100       0    -10.68562  -0.64863   4.51878  L
C-CA--0.234100       0    -9.72738   0.33452   2.4988   L
C-C-0.322600         0    -10.36571  -0.73963   3.14923  L
O-OH--0.557900       0    -10.68774  -1.86495   2.46831  L
H-H-0.271900         0    -9.00069   4.44914   7.28246  L
H-H1-0.087600        0    -10.74096   4.40244   5.117    L
H-HC-0.029500        0    -8.72154   2.4917    6.20274  L
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H-HC-0.029500        0    -8.71247   3.45728   4.76769  L
H-HA-0.169900        0    -10.55359   0.55997   6.30355  L
H-HA-0.169900        0    -8.94439   2.33396   2.72077  L
H-HA-0.165600        0    -11.17854  -1.47213   5.00636  L
H-HA-0.165600        0    -9.4852    0.24985   1.448    L
H-HO-0.399200        0    -11.59332  -2.1044    2.73381  L
N-N--0.516300        0    -11.99066   2.59705   7.48171  L
C-CT-0.038100        -1   -13.21686   2.02558   8.01531  L
C-C-0.536600         0    -14.42342   2.98043   8.17479  L
O-O--0.581900        0    -15.55714   2.48231   8.21724  L
C-CT--0.030300       0    -12.88933   1.45527   9.41934  L
C-C-0.799400         0    -12.18539   0.0931    9.40979  L
O-O2--0.801400       0    -12.69615  -0.82229   8.72524  L
O-O2--0.801400       0    -11.19064  -0.11521   10.1336  L
H-H-0.293600         0    -11.16245   2.65037   8.06723  L
H-H1-0.088000        0    -13.53398   1.21098   7.36395  L
H-HC--0.012200       0    -13.81893   1.32438   9.97522  L
H-HC--0.012200       0    -12.29363   2.1806    9.97425  L
N-N--0.415700        0    -14.18833   4.29029   8.36461  L
C-CT--0.149000       -1   -15.14133   5.3297    8.78247  L
H-H-0.271900         0    -13.23488   4.59393   8.18249  L
H-H1-0.097600        0    -16.04537   5.26155   8.17528  L
H-H1-0.097600        0    -14.68957   6.31335   8.64263  L
H-H1-0.097600        0    -15.40085   5.19289   9.83258  L
C-CT--0.366200       -1   -19.77435  -1.23151  -1.33583  L
C-C-0.597200         0    -18.77781  -0.8752   -0.22134  L
O-O--0.567900        0    -18.3935   0.28451  -0.14219  L
H-HC-0.112300        0    -20.62974  -1.75013  -0.91006  L
H-HC-0.112300        0    -19.27215  -1.86035  -2.06955  L
H-HC-0.112300        0    -20.1028  -0.31279  -1.82015  L
N-N--0.415700        0    -18.34733  -1.81842   0.64601  L
C-CT--0.058100       -1   -17.2226  -1.59484   1.60412  L
C-C-0.597300         0    -16.37268  -2.82411   1.93955  L
O-O--0.567900        0    -16.79707  -3.65001   2.7526   L
C-CT--0.007400       0    -17.66357  -0.82231   2.85841  L
C-CC-0.186800        0    -16.48087  -0.08725   3.44622  L
N-NB--0.543200       0    -15.43567  -0.69706   4.13136  L
C-CW--0.220700       0    -16.15889   1.22436   3.24181  L
C-CR-0.163500        0    -14.48087   0.23791   4.28269  L
N-NA--0.279500       0    -14.90881   1.41523   3.80262  L
H-H-0.271900         0    -18.70003  -2.7559    0.53797  L
H-H1-0.136000        0    -16.56834  -0.88808   1.09916  L
H-HC-0.036700        0    -18.0861  -1.50355   3.59731  L
H-HC-0.036700        0    -18.42364  -0.08766   2.59079  L
H-H4-0.186200        0    -16.73651   1.94123   2.67227  L
H-H-0.333900         0    -14.34277   2.2621    3.83144  L
H-H5-0.143500        0    -13.50993   0.07737   4.73779  L
N-N--0.254800        0    -15.16724  -2.94667   1.35315  L
C-CT--0.026600       -1   -14.21013  -3.96006   1.76295  L
C-C-0.589600         0    -13.52047  -3.62938   3.07685  L
O-O--0.574800        0    -13.12827  -2.4874    3.31712  L
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C-CT--0.007000       0    -13.16315  -3.99889   0.65844  L
C-CT-0.018900        0    -13.19373  -2.60592   0.03204  L
C-CT-0.019200        0    -14.63815  -2.16162   0.2365   L
H-H1-0.064100        0    -14.69768  -4.93277   1.83952  L
H-HC-0.025300        0    -13.48737  -4.73564  -0.06047  L
H-HC-0.025300        0    -12.17059  -4.25484   1.03243  L
H-HC-0.021300        0    -12.92358  -2.62515  -1.02417  L
H-HC-0.021300        0    -12.53042  -1.93569   0.57665  L
H-H1-0.039100        0    -14.64707  -1.0923    0.4494   L
H-H1-0.039100        0    -15.21624  -2.37421  -0.66429  L
N-N--0.347900        0    -13.25005  -4.64772   3.89531  L
C-CT--0.263700      -1    -12.48801  -4.46733   5.13772  L
C-C-0.734100         0    -10.97682  -4.80397   4.9649   L
O-O--0.589400        0    -10.64832  -5.65528   4.14437  L
C-CT--0.000700       0    -13.21047  -5.12162   6.32815  L
C-CT-0.039000        0    -14.53187  -4.37982   6.65475  L
C-CT-0.048600        0    -14.32431  -2.99646   7.31037  L
N-N2--0.529500       0    -15.24108  -1.95494   6.78973  L
C-CA-0.807600        0    -15.6571   -0.85827   7.40867  L
N-N2--0.862700       0    -15.37569  -0.59023   8.64339  L
N-N2--0.862700       0    -16.33184   0.05976   6.78606  L
H-H-0.274700         0    -13.51486  -5.57528   3.58888  L
H-H1-0.156000        0    -12.46765  -3.40222   5.3596   L
H-HC-0.032700        0    -12.56368  -5.10415   7.20731  L
H-HC-0.032700        0    -13.43029  -6.16174   6.08413  L
H-HC-0.028500        0    -15.11491  -4.9944    7.34127  L
H-HC-0.028500        0    -15.11977  -4.2705    5.7422   L
H-H1-0.068700        0    -13.30387  -2.66177   7.1298   L
H-H1-0.068700        0    -14.44305  -3.10303   8.39014  L
H-H-0.345600         0    -15.43037  -1.9636    5.79251  L
H-H-0.447800         0    -15.60728   0.33208   8.96827  L
H-H-0.447800         0    -14.48447  -1.00468   8.91803  L
H-H-0.447800         0    -16.41213   0.97308   7.21707  L
H-H-0.447800         0    -16.36568  -0.02606   5.77704  L
N-N--0.415700        0    -10.05408  -4.08873   5.64005  L
C-CT--0.003100      -1    -8.56741   -4.18927   5.52435  L
C-C-0.597300         0    -7.96862   -5.0261    6.66187  L
O-O--0.567900        0    -8.42681   -4.95193   7.80382  L
C-CT--0.003600       0    -7.94033   -2.78831   5.48988  L
C-CT--0.064500       0    -6.40528   -2.85695   5.40257  L
C-C-0.695100         0    -5.81907   -1.52325   4.99338  L
O-O--0.608600        0    -6.06082   -1.07527   3.88563  L
N-N--0.940700        0    -5.02799   -0.87672   5.81652  L
H-H-0.271900         0    -10.40164  -3.40569   6.30341  L
H-H1-0.085000        0    -8.33977   -4.69502   4.59214  L
H-HC-0.017100        0    -8.22669   -2.22928   6.3791   L
H-HC-0.017100        0    -8.32916   -2.2512    4.62681  L
H-HC-0.035200        0    -6.11093   -3.58821   4.65059  L
H-HC-0.035200        0    -5.99616   -3.16202   6.36312  L
H-H-0.425100         0    -4.76638    0.07857   5.60191  L
H-H-0.425100         0    -4.7045    -1.3574    6.66684  L
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N-N--0.415700        0    -6.91001  -5.77651   6.35101  L
C-CT--0.001400       -1   -6.16159  -6.59904   7.29649  L
C-C-0.597300         0    -4.6581   -6.53558   7.00593  L
O-O--0.567900        0    -4.21657  -6.70457   5.86339  L
C-CT--0.015200       0    -6.64006  -8.06265   7.23363  L
C-CA--0.001100       0    -8.1368   -8.25374   7.06833  L
C-CA--0.190600       0    -8.98249  -8.42331   8.18388  L
C-CA--0.190600       0    -8.68362  -8.2105    5.77287  L
C-CA--0.234100       0    -10.3747  -8.56426   7.99869  L
C-CA--0.234100       0    -10.06903  -8.32579   5.59367  L
C-C-0.322600         0    -10.91849  -8.5192    6.69704  L
O-OH--0.557900       0    -12.25139  -8.6667    6.48389  L
H-H-0.271900         0    -6.62302  -5.8126    5.37735  L
H-H1-0.087600        0    -6.33591  -6.22173   8.30534  L
H-HC-0.029500        0    -6.30791  -8.57702   8.13606  L
H-HC-0.029500        0    -6.15333  -8.55308   6.38884  L
H-HA-0.169900        0    -8.5648   -8.4298    9.18012  L
H-HA-0.169900        0    -8.04326  -8.04417   4.91609  L
H-HA-0.165600        0    -11.03894  -8.69468   8.83823  L
H-HA-0.165600        0    -10.49073  -8.23193   4.61103  L
H-HO-0.399200        0    -12.38989  -8.76898   5.52995  L
N-N--0.516300        0    -3.85801  -6.30749   8.04483  L
C-CT-0.039700        -1   -2.40746  -6.22454   7.9191   L
C-C-0.536600         0    -1.71444  -7.59607   7.99094  L
O-O--0.581900        0    -1.9418   -8.3881    8.90559  L
C-CT-0.056000        0    -1.79697  -5.2424    8.92638  L
C-CT-0.013600        0    -2.06782  -3.78627   8.51976  L
C-C-0.805400         0    -3.55039  -3.38624   8.61746  L
O-O2--0.818800       0    -4.24285  -3.87354   9.54462  L
O-O2--0.818800       0    -4.00529  -2.58777   7.76936  L
H-H-0.293600         0    -4.27126  -6.00626   8.91962  L
H-H1-0.110500        0    -2.19917  -5.82085   6.93468  L
H-HC--0.017300       0    -0.71435  -5.38241   8.93108  L
H-HC--0.017300       0    -2.1666   -5.44314   9.93298  L
H-HC--0.042500       0    -1.71221  -3.63903   7.49787  L
H-HC--0.042500       0    -1.46444  -3.14365   9.1606   L
N-N--0.415700        0    -0.81975  -7.86842   7.03479  L
C-CT--0.002400       -1   -0.05868  -9.12026   6.92579  L
C-C-0.597300         0     1.44371  -8.88358   7.10117  L
O-O--0.567900        0     1.9585   -7.76129   7.12781  L
C-CT--0.034300       0    -0.40274  -9.80157   5.58193  L
C-CA-0.011800        0     0.15405  -9.10999   4.34501  L
C-CA--0.125600       0    -0.57383  -8.09329   3.70134  L
C-CA--0.125600       0     1.42676  -9.45652   3.85643  L
C-CA--0.170400       0    -0.00076  -7.38152   2.63046  L
C-CA--0.170400       0     2.00336  -8.74454   2.78899  L
C-CA--0.107200       0     1.28936  -7.70063   2.17858  L
H-H-0.271900         0    -0.68301  -7.15854   6.31999  L
H-H1-0.097800        0    -0.37887  -9.78913   7.72545  L
H-HC-0.029500        0    -1.48851  -9.8679    5.49039  L
H-HC-0.029500        0    -0.0268   -10.82474   5.60397  L
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H-HA-0.133000        0    -1.55566  -7.81846   4.06333  L
H-HA-0.133000        0     1.96778  -10.26445   4.31762  L
H-HA-0.143000        0    -0.53519  -6.55883   2.17684  L
H-HA-0.143000        0     2.9944   -8.99191   2.44176  L
H-HA-0.129700        0     1.72678  -7.13021   1.3722   L
N-N--0.415700        0     2.17756  -9.98489   7.2436   L
C-CT--0.024900       -1    3.62115  -9.93452   7.43407  L
C-C-0.597300         0     4.37201  -9.43909   6.18105  L
O-O--0.567900        0     4.24767  -10.00074   5.09491  L
C-CT-0.211700        0     4.16844  -11.30966   7.85736  L
O-OH--0.654600       0     3.92511  -12.33458   6.89967  L
H-H-0.271900         0     1.69784  -10.86697   7.17991  L
H-H1-0.084300        0     3.82639  -9.23773   8.24774  L
H-H1-0.035200        0     3.71567  -11.59523   8.80844  L
H-H1-0.035200        0     5.24542  -11.22261   8.01043  L
H-HO-0.427500        0     3.15723  -12.83856   7.19818  L
N-N--0.347900        0     5.22526  -8.42199   6.32875  L
C-CT--0.263700       -1    6.11615  -7.89311   5.27151  L
C-C-0.734100         0     7.20078  -8.88696   4.82049  L
O-O--0.589400        0     7.26191  -10.02701   5.2868   L
C-CT--0.000700       0     6.67834  -6.55057   5.79045  L
C-CT-0.039000        0     7.80089  -6.6751    6.83689  L
C-CT-0.048600        0     8.14227  -5.33755   7.51025  L
N-N2--0.529500       0     8.4412   -4.25719   6.5451   L
C-CA-0.807600        0     7.6696   -3.23092   6.22941  L
N-N2--0.862700       0     6.46321  -3.1296    6.6948   L
N-N2--0.862700       0     8.07861  -2.26962   5.45907  L
H-H-0.274700         0     5.2161   -7.97411   7.23171  L
H-H1-0.156000        0     5.49773  -7.68272   4.39607  L
H-HC-0.032700        0     5.85497  -5.97214   6.21399  L
H-HC-0.032700        0     7.06529  -5.97655   4.95723  L
H-HC-0.028500        0     8.6995   -7.0581    6.35667  L
H-HC-0.028500        0     7.50113  -7.38017   7.61277  L
H-H1-0.068700        0     9.01769  -5.48922   8.14423  L
H-H1-0.068700        0     7.31816  -5.05041   8.16473  L
H-H-0.345600         0     9.37055  -4.25002   6.13213  L
H-H-0.447800         0     5.90475  -2.29935   6.45591  L
H-H-0.447800         0     6.07456  -3.79771   7.31808  L
H-H-0.447800         0     7.40754  -1.50629   5.34322  L
H-H-0.447800         0     8.97259  -2.2645    4.99427  L
N-N--0.415700        0     8.07587  -8.43815   3.92792  L
C-CT--0.051800       -1    9.41428  -8.97457   3.67092  L
C-C-0.597300         0     10.34063  -7.77228   3.84467  L
O-O--0.567900        0     10.40395  -6.88687   2.99726  L
C-CT--0.110200       0     9.43529  -9.61278   2.26618  L
C-CT-0.353100        0     10.7606  -10.27953   1.84203  L
C-CT--0.412100       0     10.47362  -11.34501   0.78095  L
C-CT--0.412100       0     11.76228  -9.30718   1.22081  L
H-H-0.271900         0     7.89018  -7.52161   3.52623  L
H-H1-0.092200        0     9.67097  -9.73597   4.40991  L
H-HC-0.045700        0     9.14307  -8.87688   1.51566  L
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H-HC-0.045700        0     8.67159  -10.38446   2.27216  L
H-HC--0.036100       0     11.21408  -10.76559   2.70606  L
H-HC-0.100000        0     11.40442  -11.8282   0.48218  L
H-HC-0.100000        0     10.01758  -10.88339  -0.09707  L
H-HC-0.100000        0     9.80584  -12.10604   1.18165  L
H-HC-0.100000        0     12.64789  -9.8506    0.89327  L
H-HC-0.100000        0     12.07072  -8.55748   1.94125  L
H-HC-0.100000        0     11.31332  -8.80842   0.36291  L
N-N--0.415700        0     11.0086  -7.69683   4.98951  L
C-CT-0.014300        -1    12.29166  -7.02058   5.02475  L
C-C-0.597300         0     13.32735  -8.08319   4.56934  L
O-O--0.567900        0     13.32004  -9.1732    5.14214  L
C-CT--0.204100       0     12.63933  -6.54358   6.4461   L
C-C-0.713000         0     11.87589  -5.32035   6.91007  L
O-O--0.593100        0     11.17547  -4.64488   6.17343  L
N-N--0.919100        0     11.98738  -4.98672   8.17361  L
H-H-0.271900         0     10.9195  -8.4783    5.62092  L
H-H1-0.104800        0     12.31915  -6.1764    4.33372  L
H-HC-0.079700        0     13.69959  -6.28656   6.46795  L
H-HC-0.079700        0     12.47983  -7.35863   7.15224  L
H-H-0.419600         0     11.52818  -4.14027   8.45299  L
H-H-0.419600         0     12.60602  -5.50107   8.77905  L
N-N--0.415700        0     14.15983  -7.83311   3.54756  L
C-CT--0.051800       -1    15.26777  -8.73831   3.18403  L
C-C-0.597300         0     16.47867  -8.51051   4.12728  L
O-O--0.567900        0     16.74239  -7.37179   4.50962  L
C-CT--0.110200       0     15.63748  -8.59115   1.67386  L
C-CT-0.353100        0     16.66084  -9.61609   1.10038  L
C-CT--0.412100       0     16.17392  -11.0579   1.28679  L
C-CT--0.412100       -1    16.94349  -9.4542   -0.41355  L
H-H-0.271900         0     14.12742  -6.93581   3.0864   L
H-H1-0.092200        0     14.92116  -9.75838   3.34519  L
H-HC-0.045700        0     16.03682  -7.59073   1.51185  L
H-HC-0.045700        0     14.72282  -8.67023   1.08775  L
H-HC--0.036100       0     17.60367  -9.50125   1.63043  L
H-HC-0.100000        0     15.1977  -11.18717   0.81995  L
H-HC-0.100000        0     16.11036  -11.30539   2.34385  L
H-HC-0.100000        0     16.88523  -11.74542   0.8283   L
H-HC-0.100000        0     16.04819  -9.67807  -0.98962  L
H-HC-0.100000        0     17.74701  -10.12792  -0.71114  L
H-HC-0.100000        0     17.26299  -8.4296   -0.60791  L
N-N--0.516300        0     17.20908  -9.56649   4.51802  L
C-CT-0.039700        -1    18.46253  -9.43774   5.30019  L
C-C-0.536600         0     19.54194  -8.62493   4.52747  L
O-O--0.581900        0     19.47397  -8.49527   3.30201  L
C-CT-0.056000        0     19.0011  -10.81021   5.74831  L
C-CT-0.013600        0     18.70294  -11.08532   7.2322   L
C-C-0.805400         0     19.25612  -10.00379   8.18202  L
O-O2--0.818800       0     18.7288  -9.91203   9.3101   L
O-O2--0.818800       0     20.14885  -9.23382   7.74999  L
H-H-0.293600         0     16.95894  -10.48018   4.18368  L
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H-H1-0.110500        0     18.22713  -8.83976   6.18144  L
H-HC--0.017300       0     20.08139  -10.85028   5.60066  L
H-HC--0.017300       0     18.56    -11.60096   5.13867  L
H-HC--0.042500       0     19.13422  -12.0532   7.49733  L
H-HC--0.042500       0     17.61923  -11.15786   7.35376  L
N-N--0.415700        0     20.50596  -8.00571   5.22698  L
C-CT--0.025200       -1    21.51064  -7.06711   4.66459  L
C-C-0.597300         0     20.89204  -5.80034   4.00711  L
O-O--0.567900        0     21.63771  -5.03041   3.40562  L
H-H-0.271900         0     20.5284  -8.22841   6.22664  L
H-H1-0.069800        0     22.09749  -7.58652   3.90719  L
H-H1-0.069800        0     22.18255  -6.74521   5.45934  L
N-N--0.415700        0     19.56617  -5.55164   4.08888  L
C-CT--0.038900       0     18.83014  -4.64776   3.16382  L
C-C-0.597300         0     17.86104  -3.65106   3.8429   L
O-O--0.567900        0     17.03999  -4.00363   4.68697  L
C-CT-0.365400        0     18.03729  -5.46969   2.12506  L
O-OH--0.676100       0     18.81359  -6.49001   1.53815  L
C-CT--0.243800       0     17.56599  -4.62218   0.94151  L
H-H-0.271900         0     19.01031  -6.21209   4.61714  L
H-H1-0.100700        0     19.56488  -4.06685   2.60776  L
H-H1-0.004300        0     17.16627  -5.91298   2.60107  L
H-HC-0.064200        0     16.903   -3.82775   1.27461  L
H-HC-0.064200        0     17.02205  -5.257     0.24181  L
H-HC-0.064200        0     18.42651  -4.18991   0.43027  L
H-HO-0.410200        0     19.04575  -7.14793   2.22088  L
N-N--0.415700        0     17.89776  -2.37797   3.42229  L
C-CT--0.087500       -1    16.98515  -1.27748   3.82932  L
C-C-0.597300         0     15.62263  -1.41615   3.11334  L
O-O--0.567900        0     15.57717  -1.42772   1.88661  L
C-CT-0.298500        0     17.57679   0.0965    3.42633  L
C-CT--0.319200       -1    16.70327   1.29482   3.89647  L
C-CT--0.319200       -1    19.02125   0.19809   3.94799  L
H-H-0.271900         0     18.57837  -2.17039   2.70697  L
H-H1-0.096900        0     16.841   -1.30796   4.90874  L
H-HC--0.029700       0     17.63648   0.14841   2.3388   L
H-HC-0.079100        0     16.58654   1.27019   4.97917  L
H-HC-0.079100        0     15.72722   1.26985   3.41263  L
H-HC-0.079100        0     17.19619   2.22625   3.61515  L
H-HC-0.079100        0     19.04617   0.02212   5.02365  L
H-HC-0.079100        0     19.40787   1.19745   3.74574  L
H-HC-0.079100        0     19.6743  -0.51488   3.44538  L
N-N--0.415700        0     14.50026  -1.52769   3.84291  L
C-CT--0.023700       -1    13.19956  -1.96538   3.27001  L
C-C-0.597300         0     11.92873  -1.33192   3.91493  L
O-O--0.567900        0     10.82541  -1.88946   3.86516  L
C-CT-0.034200        0     13.09757  -3.49843   3.49195  L
C-CT-0.001800        0     14.19085  -4.40361   2.90085  L
S-S--0.273700        0     13.72615  -5.29785   1.39462  L
C-CT--0.053600       0     13.81143  -3.94372   0.19877  L
H-H-0.271900         0     14.6375  -1.60141   4.83861  L
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 H-H1-0.088000        0     13.16415  -1.75814   2.19973  L
 H-HC-0.024100        0     12.14147  -3.8608    3.11155  L
 H-HC-0.024100        0     13.09605  -3.66729   4.56919  L
 H-H1-0.044000        0     14.44348  -5.14574   3.65745  L
 H-H1-0.044000        0     15.10137  -3.84664   2.70893  L
 H-H1-0.068400        0     14.80295  -3.49114   0.21792  L
 H-H1-0.068400        0     13.06636  -3.18726   0.44065  L
 H-H1-0.068400        0     13.61571  -4.33925  -0.7951   L
 N-N--0.415700        0     12.05602  -0.15114   4.52326  L
 C-CT--0.024900       -1    10.9386   0.75674   4.85874  L
 C-C-0.597300         0     11.02166   1.88138   3.83217  L
 O-O--0.567900        0     12.11222   2.41571   3.63261  L
 C-CT-0.211700        0     11.07539   1.22651   6.3033   L
 O-OH--0.654600       0     10.15997   2.24668   6.66059  L
 H-H-0.271900         0     12.96715   0.2766    4.43601  L
 H-H1-0.084300        0     9.98065   0.24759   4.74667  L
 H-H1-0.035200        0     12.08729   1.59404   6.43325  L
 H-H1-0.035200        0     10.92942   0.37082   6.96419  L
 H-HO-0.427500        0     9.27026   1.9971    6.307    L
 N-N--0.347900        0     9.93758   2.16889   3.09925  L
 C-CT--0.240000       -1    9.98523   3.07296   1.93425  L
 C-C-0.734100         0     10.53259   4.45918   2.35743  L
 O-O--0.589400        0     11.57416   4.83656   1.82614  L
 C-CT--0.009400       0     8.62709   3.09446   1.21793  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.65544   3.73164  -0.18575  H
 C-CT--0.047900       0     7.41914   3.28531  -0.96949  H
 C-CT--0.014300       0     7.19566   4.00375  -2.28838  H
 N-N3--0.385400       0     5.86958   3.5801   -2.85763  H
 H-H-0.274700         0     9.06869   1.6994    3.32746  L
 H-H1-0.142600        0     10.71571   2.66865   1.23154  L
 H-HC-0.036200        0     7.90758   3.62252   1.83718  L
 H-HC-0.036200        0     8.2915    2.06051   1.11515  L
 H-HC-0.010300        0     9.56958   3.42196  -0.70093  H
 H-HC-0.010300        0     8.67631   4.81993  -0.06773  H
 H-HC-0.062100        0     6.52074   3.46431  -0.38105  H
 H-HC-0.062100        0     7.45016   2.20672  -1.15598  H
 H-HP-0.113500        0     7.96363   3.81378  -3.04481  H
 H-HP-0.113500        0     7.14944   5.08479  -2.14151  H
 H-H-0.340000         0     6.00831   2.93764  -3.65054  H
 H-H-0.340000         0     5.41831   4.36546  -3.36436  H
 H-H-0.340000         0     5.14654   2.98209  -2.05801  H
 N-N--0.347900        0     9.99631   5.1203    3.41258  L
 C-CT--0.263700       -1    10.62501   6.26322   4.16728  L
 C-C-0.734100         0     11.7623   5.83331   5.06982  L
 O-O--0.589400        0     11.73714   6.08228   6.2785   L
 C-CT--0.000700       0     9.53753   7.14741   4.81216  L
 C-CT-0.039000        0     8.71732   7.83995   3.70242  L
 C-CT-0.048600        0     7.71169   8.88548   4.19429  L
 N-N2--0.529500       0     6.66759   8.33037   5.07616  L
 C-CA-0.807600        0     5.41841   8.74885   5.18251  L
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N-N2--0.862700       0     4.90716   9.64536   4.39172  L
N-N2--0.862700       0     4.67845   8.26057   6.12609  L
H-H-0.274700         0     9.09374   4.77813   3.72629  L
H-H1-0.156000        0     11.12027   6.89928   3.42679  L
H-HC-0.032700        0     10.01273   7.91849   5.4209   L
H-HC-0.032700        0     8.8893    6.54234   5.44694  L
H-HC-0.028500        0     8.18499   7.09673   3.11169  L
H-HC-0.028500        0     9.40732   8.35251   3.03066  L
H-H1-0.068700        0     7.24854   9.32228   3.30823  L
H-H1-0.068700        0     8.24563   9.67679   4.72293  L
H-H-0.345600         0     6.89028   7.56748   5.70004  L
H-H-0.447800         0     3.92229   9.91408   4.45622  L
H-H-0.447800         0     5.42474   9.93611   3.58318  L
H-H-0.447800         0     3.74826   8.65384   6.28185  L
H-H-0.447800         0     5.0197    7.52247   6.71457  L
N-N--0.347900        0     12.72315   5.1722    4.40622  L
C-CT--0.240000       -1    14.11914   4.81397   4.7239   L
C-C-0.734100         0     14.97506   4.54378   3.4547   L
O-O--0.589400        0     16.18642   4.7059    3.52506  L
C-CT--0.009400       0     14.30366   3.65245   5.74249  L
C-CT-0.018700        0     13.46533   3.94517   6.98239  L
C-CT--0.047900       0     13.52806   3.12068   8.26988  L
C-CT--0.014300       0     12.51486   3.69973   9.29321  L
N-N3--0.385400       0     11.20036   4.10469   8.70015  L
H-H-0.274700         0     12.46811   5.10656   3.42737  L
H-H1-0.142600        0     14.57685   5.69925   5.16944  L
H-HC-0.036200        0     15.35567   3.5919    6.02626  L
H-HC-0.036200        0     14.00532   2.70119   5.30391  L
H-HC-0.010300        0     12.45269   3.82668   6.61608  L
H-HC-0.010300        0     13.66746   4.97639   7.27529  L
H-HC-0.062100        0     14.53456   3.17458   8.68845  L
H-HC-0.062100        0     13.29938   2.07621   8.06865  L
H-HP-0.113500        0     12.97368   4.57982   9.7543   L
H-HP-0.113500        0     12.35946   2.95953   10.0833  L
H-H-0.340000         0     11.33675   4.85921   8.02605  L
H-H-0.340000         0     10.54464   4.42424   9.39938  L
H-H-0.340000         0     10.77604   3.3443    8.16898  L
N-N--0.415700        0     14.38472   4.11548   2.32652  L
C-CT--0.051800       -1    15.04834   3.70807   1.05858  L
C-C-0.597300         0     15.26825   4.81559   0.0642   L
O-O--0.567900        0     16.24874   4.79918  -0.67776  L
C-CT--0.110200       0     14.20153   2.55776   0.47158  L
C-CT-0.353100        0     14.74961   1.89621  -0.80824  L
C-CT--0.412100       0     16.13352   1.27812  -0.60386  L
C-CT--0.412100       0     13.79501   0.78133  -1.24411  L
H-H-0.271900         0     13.38307   3.98208   2.37298  L
H-H1-0.092200        0     16.03493   3.31523   1.30918  L
H-HC-0.045700        0     13.2044   2.944     0.2534   L
H-HC-0.045700        0     14.09728   1.785     1.23536  L
H-HC--0.036100       0     14.80065   2.63339  -1.60879  L
H-HC-0.100000        0     16.1113   0.56598   0.22018  L
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H-HC-0.100000        0     16.86337   2.05916  -0.39306  L
H-HC-0.100000        0     16.44402   0.76422  -1.51322  L
H-HC-0.100000        0     14.15041   0.34212  -2.17612  L
H-HC-0.100000        0     12.79907   1.19135  -1.40926  L
H-HC-0.100000        0     13.74748   0.00609  -0.47821  L
N-N--0.415700        0     14.35621   5.77269   0.04986  L
C-CT-0.014300       -1     14.5598    6.98748  -0.69383  L
C-C-0.597300         0     15.63205   7.91398  -0.04792  L
O-O--0.567900        0     15.32764   8.99176   0.45658  L
C-CT--0.204100       0     13.1952    7.66704  -0.97956  L
C-C-0.713000         0     12.19917   7.75915   0.17431  L
O-O--0.593100        0     12.50397   7.60783   1.34933  L
N-N--0.919100        0     10.93892   7.96381  -0.13981  L
H-H-0.271900         0     13.59169   5.74319   0.71395  L
H-H1-0.104800        0     14.9681    6.72268  -1.67091  L
H-HC-0.079700        0     12.70799   7.10633  -1.77676  L
H-HC-0.079700        0     13.37132   8.67605  -1.35086  L
H-H-0.419600         0     10.29163   7.99515   0.62147  L
H-H-0.419600         0     10.61683   8.07013  -1.10102  L
N-N--0.415700        0     16.90828   7.49487  -0.11245  L
C-CT--0.149000      -1     18.09996   8.18438   0.39861  L
H-H-0.271900         0     17.02605   6.56886  -0.51105  L
H-H1-0.097600        0     18.09276   8.16375   1.48972  L
H-H1-0.097600        0     18.0925    9.22453   0.06715  L
H-H1-0.097600        0     19.00262   7.69354   0.03285  L
C-CT--0.055800       0     0.79498   14.94928   4.41624  L
C-CT-0.000000        0     1.15189   14.05258   3.23285  L
O-OS--0.354800       0     2.54117   14.1509    2.95863  L
C-CT--0.202200       0     0.88412   12.57937   3.54848  L
O-OS--0.524600       0     0.36041   11.9917    2.35757  L
C-CT--0.067000       0     2.27585   12.06311   3.89055  L
O-OH--0.613900       0     2.35909   10.66612   3.74793  L
C-CT--0.006600       0     3.01569   12.82627   2.80703  L
N-N*--0.048400       0     4.48782   12.71892   2.92163  L
C-C-0.753800         0     5.15664   11.84669   2.05819  L
O-O--0.625200        0     4.5622    11.22194   1.1831   L
N-NC--0.758400       0     6.4939    11.65227   2.19423  L
C-CA-0.818500        0     7.13965   12.34297   3.10339  L
N-N2--0.953000       0     8.42547   12.14169   3.12432  L
C-CM--0.521500       0     6.52002   13.23504   4.01582  L
C-CM--0.005300       0     5.17696   13.39423   3.89816  L
H-H1-0.067900        0    -0.282     14.91214   4.57907  L
H-H1-0.067900        0     1.30604   14.59158   5.30999  L
H-H1-0.117400        0     0.55597   14.34741   2.36464  L
H-H1-0.061500        0     0.17925   12.48823   4.37346  L
H-H1-0.097200        0     2.57716   12.39138   4.88785  L
H-HO-0.418600        0     1.62875   10.43258   3.14663  L
H-H2-0.202900        0     2.67661   12.42669   1.84631  L
H-H-0.423400         0     8.74504   11.59059   2.34904  L
H-H-0.423400         0     9.00974   12.71172   3.70186  L
H-HA-0.192800        0     7.06163   13.77821   4.77152  L
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 H-H4-0.195800        0     4.62825   14.05574   4.55966  L
 P-P-1.166200         0    -0.56169   10.67217   2.33467  L
 O-O2--0.776000       0    -1.58793   10.79923   1.2826   L
 O-O2--0.776000       0    -0.94829   10.31334   3.71682  L
 O-OS--0.498900       0     0.48124   9.54418   1.87436  L
 C-CT-0.055800        0     1.20434   9.62525   0.65603  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     1.88891   8.27379   0.36494  H
 O-OS--0.354800       0     2.72592   7.94338   1.46571  H
 C-CT-0.202200        0     0.89446   7.12104   0.14006  H
 O-OH--0.654100       0     0.89083   6.6181   -1.18026  H
 C-CT-0.067000        0     1.3946    5.97837   1.08165  H
 O-OH--0.613900       0     1.93467   4.85384   0.41127  H
 C-CT-0.039400        0     2.56943   6.59538   1.86664  H
 N-N*--0.025100       0     2.40335   6.56152   3.29676  H
 C-CK-0.200600        0     1.52533   7.29609   4.07958  H
 N-NB--0.607300       0     1.55645   6.96463   5.34205  H
 C-CB-0.051500        0     2.48234   5.9462    5.40706  H
 C-CA-0.700900        0     2.90666   5.10877   6.45687  H
 N-N2--0.901900       0     2.45519   5.24739   7.7361   H
 N-NC--0.761500       0     3.87247   4.20993   6.209    H
 C-CQ-0.587500        0     4.23267   4.01255   4.93908  H
 N-NC--0.699700       0     3.90072   4.71777   3.86693  H
 C-CB-0.305300        0     3.02222   5.67902   4.15173  H
 H-H1-0.067900        0     1.95546   10.41126   0.73624  L
 H-H1-0.067900        0     0.52483   9.86829  -0.16367  L
 H-H1-0.117400        0     2.48833   8.36194  -0.5513   H
 H-H1-0.061500        0    -0.12122   7.41628   0.43379  H
 H-HO-0.437600        0     0.60111   7.28893  -1.83777  H
 H-H1-0.097200        0     0.59252   5.69994   1.76972  H
 H-HO-0.418600        0     5.25353   4.4547    0.88243  H
 H-H2-0.200700        0     3.47018   6.03141   1.62758  H
 H-H5-0.155300        0     0.90129   8.07072   3.64899  H
 H-H-0.411500         0     2.40503   4.36112   8.25075  H
 H-H-0.411500         0     1.57249   5.74765   7.80544  H
 H-H5-0.047300        0     4.93391   3.20428   4.76227  H
 N-N3-0.149300        0    -1.10064   4.77459  -0.2805   H
 C-CT-0.053600        0    -0.28294   3.74531   0.40847  H
 C-CT-0.065100        0    -0.87221   2.34245   0.1878   H
 C-CT--0.090300       0    -0.575     1.35537   1.32588  H
 C-C-0.735400         0    -1.50866   0.14722   1.30317  H
 O-O--0.613300        0    -1.1399   -0.99907   1.14606  H
 N-N--1.003100        0    -2.85651   0.46927   1.39254  H
 C-C-0.612300         0     1.12431   3.89447  -0.16792  H
 O-O--0.571300        0     1.54418   3.23226  -1.0662   H
 O-OS--0.421200       0     3.09033   2.0508    0.83091  H
 P-P-1.166200         0     4.21243   1.50596   0.03171  H
 O-O2--0.776000       0     5.58265   1.44021   0.87238  H
 O-O2--0.776000       0     4.52596   2.11934  -1.36679  H
 O-OS--0.498900       0     4.10541  -0.07447  -0.28671  H
 C-CT-0.055800        0     3.22071  -0.45988  -1.34074  H
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 C-CT-0.106500        0     2.59511  -1.83841  -1.04589  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.54404  -2.82373  -0.62504  L
 C-CT-0.039400        0     3.43494  -2.99178   0.79142  L
 N-N*--0.025100       0     4.78128  -2.95791   1.42063  L
 C-CB-0.305300        0     5.52394  -4.07297   1.72281  L
 N-NC--0.699700       0     5.15338  -5.37308   1.55012  L
 C-CQ-0.587500        0     6.09307  -6.21417   1.94795  L
 N-NC--0.761500       0     7.28652  -5.93846   2.45805  L
 C-CA-0.700900        0     7.6216   -4.65241   2.57341  L
 N-N2--0.901900       0     8.85301  -4.47012   3.01526  L
 C-CB-0.051500        0     6.71796  -3.62291   2.22059  L
 N-NB--0.607300       0     6.75641  -2.22479   2.25257  L
 C-CK-0.200600        0     5.57128  -1.89122   1.79636  L
 C-CT-0.067000        0     2.42475  -1.96798   1.32161  L
 O-OH--0.613900       0     1.67425  -2.44856   2.42661  L
 C-CT-0.202200        0     1.56372  -1.76935   0.07069  L
 O-OH--0.654100       0     0.61732  -2.82391  -0.08441  L
 H-H-0.199600         0    -1.79098   3.86777  -1.65014  H
 H-H-0.199600         0    -0.54206   5.50519  -0.71248  H
 H-H-0.199600         0    -1.75966   5.20491   0.36229  H
 H-HP-0.101500        0    -0.24579   3.9463    1.48856  H
 H-HC-0.005000        0    -0.51659   1.93517  -0.76436  H
 H-HC-0.005000        0    -1.95467   2.46236   0.08595  H
 H-HC-0.033100        0    -0.73563   1.85809   2.291    H
 H-HC-0.033100        0     0.45932   1.01022   1.29558  H
 H-H-0.442900         0    -3.43463  -0.29952   1.70532  H
 H-H-0.442900         0    -3.0455    1.30521   1.95981  H
 H-H1-0.067900        0     3.78282  -0.51913  -2.28119  H
 H-H1-0.067900        0     2.40797   0.2602   -1.46481  H
 H-H1-0.117400        0     2.08656  -2.15974  -1.95434  L
 H-H2-0.200700        0     2.99379  -3.9717    0.98226  L
 H-H5-0.047300        0     5.85267  -7.26226   1.84529  L
 H-H-0.411500         0     9.23168  -3.53702   3.06147  L
 H-H-0.411500         0     9.43668  -5.29913   3.06592  L
 H-H5-0.155300        0     5.25455  -0.86237   1.69443  L
 H-H1-0.097200        0     2.91064  -1.0262    1.57523  L
 H-HO-0.418600        0     2.24999  -2.52639   3.21324  L
 H-H1-0.061500        0     1.06719  -0.79968   0.07256  L
 H-HO-0.437600        0    -0.1276   -2.52632   0.47498  L
 O-OW--0.834000       0    -10.31427  -2.18497   11.53903  L
 H-HW-0.417000        0    -10.62393  -1.33865   11.13612  L
 H-HW-0.417000        0    -10.5906  -2.83806   10.87171  L
 O-OW--0.834000       0    -10.26771  -3.93694   9.4573   L
 H-HW-0.417000        0    -10.52354  -3.29169   8.77074  L
 H-HW-0.417000        0    -9.62984  -4.49995   8.97769  L
 O-OW--0.834000       0    -10.71977  -2.02643   7.61649  L
 H-HW-0.417000        0    -11.51982  -1.62471   8.04179  L
 H-HW-0.417000        0    -10.08252  -1.30862   7.69916  L
 O-OW--0.834000       0     5.40566   3.96611   1.71341  H
 H-HW-0.417000        0     4.58107   4.11064   2.23014  H
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H-HW-0.417000        0     5.61174   2.32233   1.31841  H
O-OW--0.834000       0     6.88319   4.97853   3.9367   H
H-HW-0.417000        0     6.55307   4.48724   3.15869  H
H-HW-0.417000        0     6.41041   5.81306   3.73541  H
O-OW--0.834000       0     6.49108   2.42956  -5.34124  L
H-HW-0.417000        0     7.33776   2.18075  -5.76031  L
H-HW-0.417000        0     6.26057   3.26163  -5.77887  L
O-OW--0.834000       0     6.34353   5.76208   6.53339  L
H-HW-0.417000        0     5.57034   5.23529   6.79926  L
H-HW-0.417000        0     6.56952   5.37758   5.66693  L
O-OW--0.834000       0     7.80605   1.6094    5.52905  H
H-HW-0.417000        0     7.14046   2.286     5.32679  H
H-HW-0.417000        0     7.19119   0.85039   5.74222  H
O-OW--0.834000       0     5.50868   7.01307   2.41093  H
H-HW-0.417000        0     4.90639   7.73648   2.15427  H
H-HW-0.417000        0     5.77008   6.68575   1.53305  H
O-OW--0.834000       0     3.68106   16.46738   3.88381  L
H-HW-0.417000        0     3.27711   15.64558   3.56282  L
H-HW-0.417000        0     2.93272   17.05717   3.97857  L
O-OW--0.834000       0    -4.39767   2.0887    5.82834  L
H-HW-0.417000        0    -4.25574   2.04867   6.779    L
H-HW-0.417000        0    -4.86125   2.96495   5.72982  L
O-OW--0.834000       0     0.24809   1.80546   12.15268  L
H-HW-0.417000        0    -0.14056   1.59159   13.02397  L
H-HW-0.417000        0     0.02274   2.73532   12.06858  L
O-OW--0.834000       0    -2.45912   9.93737   5.86244  L
H-HW-0.417000        0    -2.28969   9.03297   6.19669  L
H-HW-0.417000        0    -1.95363   9.97793   5.01715  L
O-OW--0.834000       0     2.16048   9.2837    6.81231  L
H-HW-0.417000        0     1.67944   8.5297    6.43063  L
H-HW-0.417000        0     1.49778   10.00314   6.72838  L
O-OW--0.834000       0    -5.03508   9.04412   5.57866  L
H-HW-0.417000        0    -4.9171    8.15468   5.96757  L
H-HW-0.417000        0    -4.17806   9.47429   5.74964  L
O-OW--0.834000       0    -2.47575   7.46835   7.04901  L
H-HW-0.417000        0    -3.31508   7.00584   6.82013  L
H-HW-0.417000        0    -2.25561   7.10649   7.92374  L
O-OW--0.834000       0     0.09115   10.91115   6.29297  L
H-HW-0.417000        0     0.10694   10.95837   5.31998  L
H-HW-0.417000        0    -0.84489   10.71568   6.45948  L
O-O2--0.818800       0     5.62715   8.03229  -0.3019   H
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**PC**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.55727 | -11.69635 | -5.51736 | L |
| C-C-0.597200 | 0 | -11.88099 | -10.68049 | -6.40909 | L |
| O-O--0.567900 | 0 | -11.50425 | -11.02902 | -7.51909 | L |
| H-HC-0.112300 | 0 | -11.94432 | -11.85538 | -4.63305 | L |
| H-HC-0.112300 | 0 | -12.65221 | -12.63159 | -6.06695 | L |
| H-HC-0.112300 | 0 | -13.54438 | -11.33001 | -5.2443 | L |
| N-N--0.415700 | 0 | -11.69738 | -9.45867 | -5.89966 | L |
| C-CT--0.058100 | -1 | -10.83622 | -8.43066 | -6.50387 | L |
| C-C-0.597300 | 0 | -9.81258 | -7.9099 | -5.48931 | L |
| O-O--0.567900 | 0 | -10.09031 | -7.83538 | -4.28585 | L |
| C-CT--0.007400 | 0 | -11.64504 | -7.33052 | -7.18654 | L |
| C-CC-0.186800 | 0 | -11.04882 | -6.84737 | -8.48284 | L |
| N-NB--0.543200 | 0 | -11.46129 | -7.24089 | -9.75545 | L |
| C-CW--0.220700 | 0 | -10.16611 | -5.81673 | -8.59859 | L |
| C-CR-0.163500 | 0 | -10.86938 | -6.38946 | -10.60602 | L |
| N-NA--0.279500 | 0 | -10.08914 | -5.52279 | -9.9413 | L |
| H-H-0.271900 | 0 | -12.05997 | -9.25944 | -4.98328 | L |
| H-H1-0.136000 | 0 | -10.26713 | -8.92126 | -7.29555 | L |
| H-HC-0.036700 | 0 | -11.7052 | -6.48192 | -6.51501 | L |
| H-HC-0.036700 | 0 | -12.65552 | -7.6848 | -7.39509 | L |
| H-H4-0.186200 | 0 | -9.72548 | -5.25233 | -7.79207 | L |
| H-H-0.333900 | 0 | -9.72886 | -4.64822 | -10.34281 | L |
| H-H5-0.143500 | 0 | -11.0564 | -6.35252 | -11.6698 | L |
| N-N--0.415700 | 0 | -8.61979 | -7.57484 | -5.97511 | L |
| C-CT--0.038900 | -1 | -7.46398 | -7.06851 | -5.2136 | L |
| C-C-0.597300 | 0 | -6.6887 | -5.99075 | -6.00712 | L |
| O-O--0.567900 | 0 | -7.0376 | -5.67953 | -7.14552 | L |
| C-CT-0.365400 | 0 | -6.47533 | -8.19825 | -4.85458 | L |
| O-OH--0.676100 | 0 | -6.1923 | -8.98446 | -5.97321 | L |
| C-CT--0.243800 | -1 | -6.98791 | -9.13841 | -3.78193 | L |
| H-H-0.271900 | 0 | -8.46301 | -7.77351 | -6.95733 | L |
| H-H1-0.100700 | 0 | -7.79827 | -6.63145 | -4.27997 | L |
| H-H1-0.004300 | 0 | -5.54473 | -7.76736 | -4.48527 | L |
| H-HC-0.064200 | 0 | -7.26239 | -8.56986 | -2.8933 | L |
| H-HC-0.064200 | 0 | -6.20943 | -9.85313 | -3.51951 | L |
| H-HC-0.064200 | 0 | -7.86355 | -9.67539 | -4.14755 | L |
| H-HO-0.410200 | 0 | -5.47538 | -9.60459 | -5.76281 | L |
| N-N--0.347900 | 0 | -5.61097 | -5.41408 | -5.43828 | L |
| C-CT--0.263700 | -1 | -4.63092 | -4.55998 | -6.15734 | L |
| C-C-0.734100 | 0 | -3.2308 | -4.60386 | -5.55647 | L |
| O-O--0.589400 | 0 | -3.11161 | -4.80964 | -4.35324 | L |
| C-CT--0.000700 | 0 | -5.15288 | -3.10785 | -6.27494 | L |
| C-CT-0.039000 | 0 | -4.97563 | -2.15652 | -5.07035 | L |
| C-CT-0.048600 | 0 | -5.74681 | -2.48046 | -3.78673 | L |
| N-N2--0.529500 | 0 | -5.11681 | -3.5263 | -2.97359 | L |
| C-CA-0.807600 | 0 | -5.06109 | -3.596 | -1.66228 | L |
| N-N2--0.862700 | 0 | -5.72365 | -2.81551 | -0.8624 | L |
| N-N2--0.862700 | 0 | -4.29388 | -4.49454 | -1.13094 | L |
| H-H-0.274700 | 0 | -5.37493 | -5.71998 | -4.50634 | L |
| H-H1-0.156000 | 0 | -4.56298 | -4.97026 | -7.16064 | L |

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 H-HC-0.032700        0    -6.20781  -3.12593  -6.55216  L
 H-HC-0.032700        0    -4.62788  -2.64668  -7.11308  L
 H-HC-0.028500        0    -5.3459   -1.18442  -5.38722  L
 H-HC-0.028500        0    -3.918    -2.03316  -4.83995  L
 H-H1-0.068700        0    -6.76691  -2.75742  -4.04494  L
 H-H1-0.068700        0    -5.77095  -1.56429  -3.19586  L
 H-H-0.345600         0    -4.47771  -4.14517  -3.44898  L
 H-H-0.447800         0    -5.73739  -2.93558   0.13878  L
 H-H-0.447800         0    -6.44134  -2.19133  -1.25475  L
 H-H-0.447800         0    -3.99684  -4.35673  -0.17157  L
 H-H-0.447800         0    -3.86004  -5.19911  -1.71959  L
 N-N--0.415700        0    -2.17981  -4.31308  -6.31658  L
 C-CT--0.002400      -1    -0.93872  -3.7916   -5.72255  L
 C-C-0.597300         0    -0.99321  -2.2536   -5.70442  L
 O-O--0.567900        0    -1.11993  -1.66219  -6.77755  L
 C-CT--0.034300       0     0.29171  -4.28901  -6.48732  L
 C-CA-0.011800        0     1.58353  -3.68311  -5.96402  L
 C-CA--0.125600       0     2.03995  -3.97978  -4.66342  L
 C-CA--0.125600       0     2.30727  -2.77847  -6.76226  L
 C-CA--0.170400       0     3.20094  -3.35837  -4.16572  L
 C-CA--0.170400       0     3.46879  -2.16464  -6.2672   L
 C-CA--0.107200       0     3.90391  -2.43673  -4.96146  L
 H-H-0.271900         0    -2.36718  -4.17049  -7.30514  L
 H-H1-0.097800        0    -0.83583  -4.16347  -4.70515  L
 H-HC-0.029500        0     0.17757  -4.04215  -7.54433  L
 H-HC-0.029500        0     0.35045  -5.37417  -6.39616  L
 H-HA-0.133000        0     1.49064  -4.66852  -4.03764  L
 H-HA-0.133000        0     1.96233  -2.53344  -7.75402  L
 H-HA-0.143000        0     3.54776  -3.57122  -3.16583  L
 H-HA-0.143000        0     4.01571  -1.46932  -6.88625  L
 H-HA-0.129700        0     4.77451  -1.9255   -4.57573  L
 N-N--0.254800        0    -0.94129  -1.60708  -4.52461  L
 C-CT--0.026600       0    -0.7791   -0.16281  -4.39897  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.71829   0.22613  -4.23641  H
 O-O--0.574800        0     1.33811   0.03333  -3.2011   H
 C-CT--0.007000       0    -1.58283   0.18288  -3.14692  L
 C-CT-0.018900        0    -1.39703  -1.03063  -2.24112  L
 C-CT-0.019200        0    -1.21548  -2.1934   -3.21552  L
 H-H1-0.064100        0    -1.22461   0.36126  -5.24171  L
 H-HC-0.025300        0    -2.63519   0.27995  -3.41148  L
 H-HC-0.025300        0    -1.21789   1.0903   -2.67278  L
 H-HC-0.021300        0    -2.26269  -1.18051  -1.59502  L
 H-HC-0.021300        0    -0.4957   -0.90379  -1.64598  L
 H-H1-0.039100        0    -0.38871  -2.82575  -2.88935  L
 H-H1-0.039100        0    -2.13937  -2.76845  -3.25234  L
 N-N--0.254800        0     1.34576   0.80869  -5.29595  H
 C-CT--0.026600       0     2.56983   1.54695  -5.08948  H
 C-C-0.589600         0     2.22953   2.9691   -4.60676  H
 O-O--0.574800        0     1.09726   3.41894  -4.72753  H
 C-CT--0.007000       0     3.13265   1.6719   -6.51306  H
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 C-CT-0.018900        0     1.86531   1.9178   -7.33946  H
 C-CT-0.019200        0     0.75867   1.14695  -6.59435  H
 H-H1-0.064100        0     3.23496   1.04     -4.38776  H
 H-HC-0.025300        0     3.62848   0.74265  -6.7937   H
 H-HC-0.025300        0     3.85389   2.48771  -6.60275  H
 H-HC-0.021300        0     1.95981   1.58998  -8.37529  H
 H-HC-0.021300        0     1.63767   2.98513  -7.34091  H
 H-H1-0.039100        0    -0.12836   1.77067  -6.46008  H
 H-H1-0.039100        0     0.49016   0.23196  -7.12832  H
 N-N--0.415700        0     3.2953    3.63856  -4.11919  H
 C-CT-0.039700        0     3.43434   5.0904   -4.04104  H
 C-C-0.597300         0     4.34553   5.47046  -5.25378  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.47537   4.98501  -5.31829  L
 C-CT--0.003600       0     3.90625   5.35789  -2.59138  H
 C-CT-0.013600        0     4.42747   6.7299   -2.19773  H
 C-C-0.805400         0     5.03364   6.71064  -0.79904  H
 O-O2--0.818800       0     5.32805   5.68719  -0.18846  H
 H-H-0.271900         0     4.20618   3.19343  -4.14471  H
 H-H1-0.110500        0     2.4532    5.54309  -4.19681  H
 H-HC--0.017300       0     3.04824   5.11855  -1.95423  H
 H-HC--0.017300       0     4.66459   4.62017  -2.32468  H
 H-HC--0.042500       0     3.64221   7.49365  -2.21723  H
 H-HC--0.042500       0     5.22137   7.07815  -2.86865  H
 N-N--0.254800        0     3.86987   6.16906  -6.31009  L
 C-CT--0.026600       -1    4.66018   6.60608  -7.48746  L
 C-C-0.589600         0     6.06743   7.17158  -7.19878  L
 O-O--0.574800        0     6.9506    7.08056  -8.05308  L
 C-CT--0.007000       0     3.73439   7.52479  -8.27764  L
 C-CT-0.018900        0     2.38574   6.85649  -8.02862  L
 C-CT-0.019200        0     2.46745   6.48192  -6.5488   L
 H-H1-0.064100        0     4.81317   5.72117  -8.0989   L
 H-HC-0.025300        0     3.98831   7.55643  -9.33746  L
 H-HC-0.025300        0     3.72549   8.51627  -7.84044  L
 H-HC-0.021300        0     2.31229   5.95227  -8.6301   L
 H-HC-0.021300        0     1.55069   7.5157   -8.24611  L
 H-H1-0.039100        0     2.16977   7.32806  -5.92914  L
 H-H1-0.039100        0     1.82562   5.62438  -6.34931  L
 N-N--0.415700        0     6.33876   7.66661  -5.98793  L
 C-CT-0.014300        -1    7.68698   7.83292  -5.4483   L
 C-C-0.597300         0     8.48464   6.53617  -5.41106  L
 O-O--0.567900        0     8.2696    5.65892  -4.57631  L
 C-CT--0.204100       0     7.63608   8.47211  -4.0465   L
 C-C-0.713000         0     9.01396   8.89354  -3.55849  L
 O-O--0.593100        0     9.65443   8.25468  -2.73402  L
 N-N--0.919100        0     9.54141   9.98297  -4.06111  L
 H-H-0.271900         0     5.52265   7.86186  -5.40674  L
 H-H1-0.104800        0     8.2053    8.53121  -6.10755  L
 H-HC-0.079700        0     7.23268   7.759    -3.33206  L
 H-HC-0.079700        0     6.98606   9.34052  -4.0637   L
 H-H-0.419600         0     10.44199   10.24221  -3.71058  L
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H-H-0.419600          0     9.03963   10.56664  -4.72951  L
N-N--0.415700         0     9.51285   6.47924  -6.24204  L
C-CT--0.025200        -1    10.68264   5.69152  -5.92422  L
C-C-0.597300          0     11.04582   4.68609  -7.02159  L
O-O--0.567900         0     11.58033   5.03546  -8.06933  L
H-H-0.271900          0     9.5561    7.15326  -6.99286  L
H-H1-0.069800         0     10.56557   5.16478  -4.97672  L
H-H1-0.069800         0     11.52854   6.36939  -5.81319  L
N-N--0.415700         0     10.77872   3.4217   -6.72181  L
C-CT--0.001400        -1    10.82283   2.2146   -7.5587   L
C-C-0.597300          0     9.77483   1.28374  -6.92785  L
O-O--0.567900         0     8.95754   1.72958  -6.11298  L
C-CT--0.015200        0     12.26053   1.64949  -7.55788  L
C-CA--0.001100        0     12.76178   1.25147  -8.93169  L
C-CA--0.190600        0     13.18189   2.25603  -9.82562  L
C-CA--0.190600        0     12.82664  -0.10263  -9.31466  L
C-CA--0.234100        0     13.6739   1.91247  -11.09948  L
C-CA--0.234100        0     13.30953  -0.44995  -10.59123  L
C-C-0.322600          0     13.73599   0.55519  -11.48355  L
O-OH--0.557900        0     14.19647   0.21558  -12.71561  L
H-H-0.271900          0     10.25463   3.29735  -5.86675  L
H-H1-0.087600         0     10.5149   2.46077  -8.57654  L
H-HC-0.029500         0     12.34147   0.80468  -6.87298  L
H-HC-0.029500         0     12.94785   2.40904  -7.18108  L
H-HA-0.169900         0     13.11932   3.29608  -9.5278   L
H-HA-0.169900         0     12.51047  -0.88164  -8.63563  L
H-HA-0.165600         0     13.99197   2.68866  -11.77754  L
H-HA-0.165600         0     13.35777  -1.48274  -10.9008  L
H-HO-0.399200         0     14.45412   0.99095  -13.21404  L
N-N--0.415700         0     9.85418  -0.01342  -7.16807  L
C-CT--0.051800        -1    9.40221  -1.00239  -6.19421  L
C-C-0.597300          0     10.5474  -1.95606  -5.8976   L
O-O--0.567900         0     11.50464  -2.08747  -6.66031  L
C-CT--0.110200        0     8.09377  -1.65874  -6.68759  L
C-CT-0.353100         0     8.12186  -2.35764  -8.06383  L
C-CT--0.412100        0     8.67775  -3.78264  -7.98262  L
C-CT--0.412100        0     6.69463  -2.44629  -8.60649  L
H-H-0.271900          0     10.47708  -0.31832  -7.90462  L
H-H1-0.092200         0     9.18433  -0.49144  -5.2595   L
H-HC-0.045700         0     7.34946  -0.86138  -6.72537  L
H-HC-0.045700         0     7.74614  -2.37442  -5.94384  L
H-HC--0.036100        0     8.71644  -1.78293  -8.77197  L
H-HC-0.100000         0     9.73102  -3.76078  -7.71371  L
H-HC-0.100000         0     8.58916  -4.26111  -8.95804  L
H-HC-0.100000         0     8.12284  -4.36359  -7.24671  L
H-HC-0.100000         0     6.06079  -3.00682  -7.924    L
H-HC-0.100000         0     6.69573  -2.92561  -9.58644  L
H-HC-0.100000         0     6.28413  -1.44535  -8.71622  L
N-N--0.415700         0     10.48203  -2.56581  -4.72817  L
C-CT--0.058100        -1    11.57215  -3.34026  -4.14934  L
C-C-0.597300          0     11.07399  -4.73232  -3.78448  L
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 O-O--0.567900        0     9.87613  -5.00593  -3.77733  L
 C-CT--0.007400       0     12.12868  -2.56486  -2.94111  L
 C-CC-0.186800        0     11.09951  -2.22969  -1.88273  L
 N-NB--0.543200       0     10.74462  -3.03792  -0.80249  L
 C-CW--0.220700       0     10.32252  -1.10902  -1.86602  L
 C-CR-0.163500        0     9.77055  -2.37896  -0.15119  L
 N-NA--0.279500       0     9.48382  -1.22789  -0.7789   L
 H-H-0.271900         0     9.63376  -2.43178  -4.19029  L
 H-H1-0.136000        0     12.37075  -3.46263  -4.88315  L
 H-HC-0.036700        0     12.56251  -1.63096  -3.30124  L
 H-HC-0.036700        0     12.93378  -3.13782  -2.4867   L
 H-H4-0.186200        0     10.32753  -0.31762  -2.60322  L
 H-H-0.333900         0     8.7001   -0.62436  -0.55291  L
 H-H5-0.143500        0     9.24858  -2.74064   0.72622  L
 N-N--0.415700        0     11.9863  -5.64768  -3.47724  L
 C-CT--0.059700       -1    11.58911  -7.0205   -3.16225  L
 C-C-0.597300         0     10.67068  -7.14121  -1.92003  L
 O-O--0.567900        0     9.91086  -8.10128  -1.80735  L
 C-CT-0.130300        0     12.82181  -7.93489  -3.05934  L
 C-CT--0.043000       0     12.35937  -9.40403  -2.96864  L
 C-CT--0.320400       0     13.74588  -7.55075  -1.88825  L
 C-CT--0.066000       -1    13.42454  -10.38606  -3.43309  L
 H-H-0.271900         0     12.96407  -5.40607  -3.51509  L
 H-H1-0.086900        0     11.00558  -7.37652  -4.00884  L
 H-HC-0.018700        0     13.38568  -7.81488  -3.98659  L
 H-HC-0.023600        0     11.49055  -9.55389  -3.6104   L
 H-HC-0.023600        0     12.07472  -9.64751  -1.94409  L
 H-HC-0.088200        0     14.64854  -8.15773  -1.92048  L
 H-HC-0.088200        0     13.24684  -7.71464  -0.93234  L
 H-HC-0.088200        0     14.04698  -6.50668  -1.95877  L
 H-HC-0.018600        0     13.02763  -11.40016  -3.37878  L
 H-HC-0.018600        0     14.30505  -10.32009  -2.79442  L
 H-HC-0.018600        0     13.70645  -10.17196  -4.46461  L
 N-N--0.415700        0     10.68353  -6.16202  -1.00798  L
 C-CT--0.025200       -1    9.65419  -6.02235   0.02357  L
 C-C-0.597300         0     8.26324  -5.90824  -0.59895  L
 O-O--0.567900        0     7.4534   -6.82825  -0.47147  L
 H-H-0.271900         0     11.30223  -5.37797  -1.15311  L
 H-H1-0.069800        0     9.85571  -5.14663   0.63587  L
 H-H1-0.069800        0     9.66779  -6.90312   0.66038  L
 N-N--0.415700        0     8.01341  -4.82135  -1.34132  L
 C-CT--0.058100       0     6.81689  -4.6502   -2.18234  L    H-HC
246   0.        0.
 C-C-0.597300         0     6.47142  -5.92344  -2.97191  L
 O-O--0.567900        0     5.30225  -6.29531  -3.0363   L
 C-CT--0.007400       0     6.99538  -3.49139  -3.16834  H
 C-CC-0.186800        0     6.97035  -2.06782  -2.70801  H
 N-NB--0.543200       0     7.53897  -1.15049  -3.55703  H
 C-CW--0.220700       0     6.31242  -1.4203   -1.69554  H
 C-CR-0.163500        0     7.17379   0.02716  -3.10869  H
 N-NA--0.279500       0     6.45134  -0.07379  -1.96425  H
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H-H-0.271900          0     8.77183  -4.15908  -1.45145  L
H-H1-0.136000         0     5.957    -4.43114  -1.54594  L
H-HC-0.036700         0     6.20082  -3.59482  -3.91649  H
H-HC-0.036700         0     7.91752  -3.63237  -3.72717  H
H-H4-0.186200         0     5.73537  -1.75792  -0.8542   H
H-H-0.333900          0     5.93423   0.69638  -1.54584  H
H-H5-0.143500         0     7.3934    0.98523  -3.56737  H
N-N--0.415700         0     7.4672   -6.61757  -3.53858  L
C-CT-0.033700         -1    7.28038  -7.87575  -4.26402  L
C-C-0.597300          0     6.47445  -8.9417   -3.51681  L
O-O--0.567900         0     5.65242  -9.61618  -4.13692  L
C-CT--0.182500        0     8.59984  -8.4087   -4.82672  L
H-H-0.271900          0     8.39382  -6.20849  -3.49005  L
H-H1-0.082300         0     6.67165  -7.62315  -5.13042  L
H-HC-0.060300         0     9.14681  -7.60392  -5.31914  L
H-HC-0.060300         0     8.38586  -9.18495  -5.56263  L
H-HC-0.060300         0     9.1999   -8.84971  -4.03626  L
N-N--0.347900         0     6.63934  -9.08014  -2.19657  L
C-CT--0.240000        -1    5.75148  -9.93788  -1.4014   L
C-C-0.734100          0     4.2757   -9.48522  -1.46381  L
O-O--0.589400         0     3.40101  -10.33262  -1.62248  L
C-CT--0.009400        0     6.26497  -10.07919   0.04088  L
C-CT-0.018700         0     5.37275  -11.02115   0.8753   L
C-CT--0.047900        0     5.99238  -11.31842   2.24458  L
C-CT--0.014300        0     5.02641  -12.09008   3.15118  L
N-N3--0.385400        0     5.60728  -12.29205   4.50338  L
H-H-0.274700          0     7.31301  -8.46605  -1.74334  L
H-H1-0.142600         0     5.76646  -10.93085  -1.8542   L
H-HC-0.036200         0     6.29884  -9.09869   0.5144   L
H-HC-0.036200         0     7.27866  -10.48187   0.00764  L
H-HC-0.010300         0     5.23035  -11.96097   0.3394   L
H-HC-0.010300         0     4.40026  -10.55157   1.02712  L
H-HC-0.062100         0     6.2356   -10.36875   2.71976  L
H-HC-0.062100         0     6.90376  -11.90115   2.10311  L
H-HP-0.113500         0     4.77189  -13.04783   2.68843  L
H-HP-0.113500         0     4.10771  -11.50013   3.24193  L
H-H-0.340000          0     4.88772  -12.55164   5.17392  L
H-H-0.340000          0     5.96111  -11.40018   4.85056  L
H-H-0.340000          0     6.35987  -12.96194   4.50685  L
N-N--0.415700         0     3.98836  -8.1843   -1.33674  L
C-CT--0.024900        -1    2.63853  -7.6059   -1.51701  L
C-C-0.597300          0     2.08807  -7.8777   -2.92734  L
O-O--0.567900         0     0.96305  -8.36062  -3.02707  L
C-CT-0.211700         0     2.63206  -6.09927  -1.19811  L
O-OH--0.654600        0     1.29888  -5.63953  -1.07528  L
H-H-0.271900          0     4.77681  -7.55171  -1.29379  L
H-H1-0.084300         0     1.96635  -8.09282  -0.80977  L
H-H1-0.035200         0     3.1394   -5.54323  -1.98538  L
H-H1-0.035200         0     3.15154  -5.93034  -0.25485  L
H-HO-0.427500         0     1.28202  -4.70336  -0.8012   L
N-N--0.415700         0     2.86551  -7.65248  -4.00416  L
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C-CT--0.059700       -1    2.5389   -8.0835   -5.39056  L
C-C-0.597300         0     2.12242  -9.57236  -5.36217  L
O-O--0.567900        0     0.99552  -9.89155  -5.7212   L
C-CT-0.130300        0     3.69253  -7.80755  -6.38618  L
C-CT--0.043000       0     4.06909  -6.30973  -6.40209  L
C-CT--0.320400       0     3.30026  -8.25995  -7.80541  L
C-CT--0.066000       0     5.30312  -5.97718  -7.24755  L
H-H-0.271900         0     3.76489  -7.21557  -3.8286   L
H-H1-0.086900        0     1.66916  -7.51528  -5.72258  L
H-HC-0.018700        0     4.56546  -8.38025  -6.07889  L
H-HC-0.023600        0     4.28031  -5.97682  -5.3886   L
H-HC-0.023600        0     3.22598  -5.73012  -6.7758   L
H-HC-0.088200        0     2.46966  -7.65861  -8.17697  L
H-HC-0.088200        0     3.01183  -9.31108  -7.81793  L
H-HC-0.088200        0     4.14423  -8.14743  -8.48534  L
H-HC-0.018600        0     5.05551  -6.00926  -8.30863  L
H-HC-0.018600        0     6.11027  -6.67841  -7.04184  L
H-HC-0.018600        0     5.6379   -4.97388  -6.99388  L
N-N--0.415700        0     2.98382  -10.48235  -4.88843  L
C-CT-0.021300        -1    2.75826  -11.94084  -4.89274  L
C-C-0.597300         0     1.53399  -12.44136  -4.12756  L
O-O--0.567900        0     0.98293  -13.4786  -4.48156  L
C-CT--0.123100       -1    4.06608  -12.67948  -4.47529  L
S-SH--0.311900       0     5.41199  -12.346   -5.6484   L
H-H-0.271900         0     3.88879  -10.14493  -4.58381  L
H-H1-0.112400        0     2.56187  -12.22474  -5.92858  L
H-H1-0.111200        0     3.86998  -13.75361  -4.46651  L
H-H1-0.111200        0     4.35899  -12.36678  -3.47222  L
H-HS-0.193300        0     5.57734  -11.05267  -5.3323   L
N-N--0.415700        0     1.10559  -11.73213  -3.08789  L
C-CT--0.051800       -1   -0.12938  -12.03867  -2.37226  L
C-C-0.597300         0    -1.35814  -11.39525  -3.04094  L
O-O--0.567900        0    -2.33461  -12.09907  -3.27377  L
C-CT--0.110200       0     0.01528  -11.5626  -0.91549  L
C-CT-0.353100        0     1.03175  -12.38804  -0.10244  L
C-CT--0.412100       0     1.37478  -11.65799   1.19402  L
C-CT--0.412100       0     0.48935  -13.77088   0.26615  L
H-H-0.271900         0     1.64781  -10.91733  -2.82805  L
H-H1-0.092200        0    -0.30194  -13.11564  -2.37857  L
H-HC-0.045700        0    -0.95673  -11.62041  -0.42336  L
H-HC-0.045700        0     0.32264  -10.51502  -0.92203  L
H-HC--0.036100       0     1.95438  -12.51458  -0.66793  L
H-HC-0.100000        0     1.82273  -10.69752   0.9431   L
H-HC-0.100000        0     2.08248  -12.24381   1.77579  L
H-HC-0.100000        0     0.46861  -11.48678   1.77696  L
H-HC-0.100000        0     1.22115  -14.31095   0.86454  L
H-HC-0.100000        0     0.29537  -14.34683  -0.63834  L
H-HC-0.100000        0    -0.43914  -13.67169   0.82933  L
N-N--0.415700        0    -1.3299   -10.09419  -3.37091  L
C-CT-0.014300        -1   -2.42754  -9.40239  -4.0755   L
C-C-0.597300         0    -2.78496  -10.09491  -5.37612  L
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O-O--0.567900        0    -3.93399  -10.4897  -5.57816  L
C-CT--0.204100       0    -2.15184  -7.89956  -4.19721  L
C-C-0.713000         0    -2.36308  -7.19827  -2.86401  L
O-O--0.593100        0    -3.47451  -6.88887  -2.45941  L
N-N--0.919100        0    -1.31436  -6.92818  -2.12735  L
H-H-0.271900         0    -0.47464  -9.58075  -3.19218  L
H-H1-0.104800        0    -3.32244  -9.50807  -3.45711  L
H-HC-0.079700        0    -2.86366  -7.47281  -4.90217  L
H-HC-0.079700        0    -1.14707  -7.71774  -4.57631  L
H-H-0.419600         0    -1.44317  -6.41305  -1.27718  L
H-H-0.419600         0    -0.39457  -7.21283  -2.43605  L
N-N--0.415700        0    -1.7714   -10.32662  -6.19861  L
C-CT--0.002400       -1   -1.91025  -11.15112  -7.37737  L
C-C-0.597300         0    -2.10162  -12.64478  -7.12812  L
O-O--0.567900        0    -2.58639  -13.35484  -8.00358  L
C-CT--0.034300       0    -0.77221  -10.86816  -8.37362  L
C-CA-0.011800        0    -0.90164  -9.51802  -9.06336  L
C-CA--0.125600       0    -1.63257  -9.41504  -10.26296  L
C-CA--0.125600       0    -0.34998  -8.35514  -8.49092  L
C-CA--0.170400       0    -1.82525  -8.1619   -10.87255  L
C-CA--0.170400       0    -0.53278  -7.1031   -9.10683  L
C-CA--0.107200       0    -1.27871  -7.00462  -10.29327  L
H-H-0.271900         0    -0.84794  -9.98827  -5.95397  L
H-H1-0.097800        0    -2.82905  -10.84237  -7.87921  L
H-HC-0.029500        0    -0.78927  -11.63738  -9.14716  L
H-HC-0.029500        0     0.1931   -10.94521  -7.87594  L
H-HA-0.133000        0    -2.07741  -10.29514  -10.70488  L
H-HA-0.133000        0     0.19418  -8.41625  -7.56412  L
H-HA-0.143000        0    -2.41848  -8.08024  -11.77395  L
H-HA-0.143000        0    -0.12257  -6.2091   -8.66368  L
H-HA-0.129700        0    -1.44771  -6.03987  -10.75318  L
N-N--0.415700        0    -1.76654  -13.11367  -5.93226  L
C-CT--0.025200       -1   -1.98088  -14.48312  -5.49622  L
C-C-0.597300         0    -3.44147  -14.89611  -5.35172  L
O-O--0.567900        0    -3.79548  -16.03269  -5.65124  L
H-H-0.271900         0    -1.39589  -12.46281  -5.25885  L
H-H1-0.069800        0    -1.49474  -14.62714  -4.53219  L
H-H1-0.069800        0    -1.51202  -15.15813  -6.21264  L
N-N--0.415700        0    -4.2772   -13.9831  -4.85936  L
C-CT--0.059700       -1   -5.73737  -14.14023  -4.79678  L
C-C-0.597300         0    -6.39862  -14.1061  -6.17802  L
O-O--0.567900        0    -7.412    -14.77216  -6.38386  L
C-CT-0.130300        0    -6.2966   -13.08902  -3.78173  L
C-CT--0.043000       0    -5.97143  -13.57009  -2.32734  L
C-CT--0.320400       -1   -7.81189  -12.76629  -3.93833  L
C-CT--0.066000       -1   -5.29235  -12.55696  -1.37565  L
H-H-0.271900         0    -3.86577  -13.10127  -4.57732  L
H-H1-0.086900        0    -5.96179  -15.13336  -4.40564  L
H-HC-0.018700        0    -5.76264  -12.15366  -3.9576   L
H-HC-0.023600        0    -5.30908  -14.43566  -2.36863  L
H-HC-0.023600        0    -6.89167  -13.91641  -1.85514  L
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H-HC-0.088200        0    -7.99603  -12.29467  -4.90574  L
H-HC-0.088200        0    -8.12637  -12.07665  -3.15509  L
H-HC-0.088200        0    -8.39807  -13.68366  -3.87406  L
H-HC-0.018600        0    -4.33942  -12.23661  -1.78735  L
H-HC-0.018600        0    -5.12596  -13.02109  -0.40344  L
H-HC-0.018600        0    -5.93819  -11.68736  -1.25374  L
N-N--0.415700        0    -5.80376  -13.37765  -7.12584  L
C-CT--0.149000       -1   -6.20218  -13.38073  -8.52169  L
H-H-0.271900         0    -4.96667  -12.88198  -6.86203  L
H-H1-0.097600        0    -6.47835  -14.3915  -8.82761  L
H-H1-0.097600        0    -5.37568  -13.03141  -9.14179  L
H-H1-0.097600        0    -7.06266  -12.72124  -8.65503  L
C-CT--0.366200       -1   -8.63358  -10.25589  -10.70441  L
C-C-0.597200         0    -7.88515  -9.56407  -9.63141  L
O-O--0.567900        0    -8.23997  -9.57708  -8.46033  L
H-HC-0.112300        0    -7.99378  -10.98246  -11.19955  L
H-HC-0.112300        0    -9.01456  -9.5193   -11.41014  L
H-HC-0.112300        0    -9.48122  -10.76782  -10.24729  L
N-N--0.415700        0    -6.82326  -8.94504  -10.091   L
C-CT-0.021300        -1   -6.0331   -8.06674  -9.28745  L
C-C-0.597300         0    -5.54053  -6.91437  -10.16187  L
O-O--0.567900        0    -4.94093  -7.17201  -11.20932  L
C-CT--0.123100       0    -4.83163  -8.848    -8.73399  L
S-SH--0.311900       0    -3.75854  -7.74974  -7.75167  L
H-H-0.271900         0    -6.63673  -8.96658  -11.08068  L
H-H1-0.112400        0    -6.62287  -7.67476  -8.45986  L
H-H1-0.111200        0    -4.26029  -9.26555  -9.56242  L
H-H1-0.111200        0    -5.19296  -9.66923  -8.11472  L
H-HS-0.193300        0    -3.2731   -7.04184  -8.78498  L
N-N--0.415700        0    -5.7592   -5.66689  -9.7433   L
C-CT-0.014300        -1   -5.29808  -4.50459  -10.49813  L
C-C-0.597300         0    -3.91871  -3.96126  -10.02056  L
O-O--0.567900        0    -3.35478  -4.39769  -9.01319  L
C-CT--0.204100       0    -6.41927  -3.44967  -10.58436  L
C-C-0.713000         0    -6.23186  -2.46734  -11.73908  L
O-O--0.593100        0    -5.40158  -2.65544  -12.61848  L
N-N--0.919100        0    -6.94866  -1.37809  -11.77468  L
H-H-0.271900         0    -6.28155  -5.5294   -8.88308  L
H-H1-0.104800        0    -5.12948  -4.83547  -11.52468  L
H-HC-0.079700        0    -6.49802  -2.90016  -9.64684  L
H-HC-0.079700        0    -7.35881  -3.96687  -10.7647  L
H-H-0.419600         0    -6.80763  -0.76416  -12.54773  L
H-H-0.419600         0    -7.74754  -1.24742  -11.13955  L
N-N--0.415700        0    -3.34747  -2.99709  -10.74455  L
C-CT--0.051800       -1   -2.23727  -2.13537  -10.32716  L
C-C-0.597300         0    -2.83026  -0.7262   -10.05642  L
O-O--0.567900        0    -3.15848  -0.01471  -11.00471  L
C-CT--0.110200       0    -1.1605   -2.12773  -11.43086  L
C-CT-0.353100        0    -0.01246  -1.12154  -11.20794  L
C-CT--0.412100       0     0.78135  -1.41871  -9.93664  L
C-CT--0.412100       0     0.96529  -1.19168  -12.38365  L
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H-H-0.271900          0    -3.86325  -2.70134  -11.57027  L
H-H1-0.092200         0    -1.79516  -2.50737  -9.40257  L
H-HC-0.045700         0    -1.6441   -1.88101  -12.37784  L
H-HC-0.045700         0    -0.74536  -3.13239  -11.51766  L
H-HC--0.036100        0    -0.40727  -0.10918  -11.15214  L
H-HC-0.100000         0     1.1551   -2.44108  -9.96076  L
H-HC-0.100000         0     0.13957  -1.2753   -9.06828  L
H-HC-0.100000         0     1.61118  -0.71808  -9.85249  L
H-HC-0.100000         0     1.39028  -2.19215  -12.45979  L
H-HC-0.100000         0     1.76229  -0.46461  -12.2346  L
H-HC-0.100000         0     0.43498  -0.94989  -13.30462  L
N-N--0.347900         0    -3.00229  -0.33108  -8.781    L
C-CT--0.263700        -1   -3.38986   1.04897  -8.37805  L
C-C-0.734100          0    -2.16553   1.95776  -8.52746  L
O-O--0.589400         0    -1.05956   1.48733  -8.78895  L
C-CT--0.000700        0    -3.99568   1.01289  -6.96867  L
C-CT-0.039000         0    -4.79667   2.27637  -6.62109  L
C-CT-0.048600         0    -5.61936   2.09451  -5.34888  L
N-N2--0.529500        0    -4.77976   1.96776  -4.15244  L
C-CA-0.807600         0    -5.23894   1.81074  -2.93053  L
N-N2--0.862700        0    -6.47368   1.52971  -2.67772  L
N-N2--0.862700        0    -4.47471   1.9444   -1.89753  L
H-H-0.274700          0    -2.59043  -0.92943  -8.0758   L
H-H1-0.156000         0    -4.14321   1.40574  -9.08338  L
H-HC-0.032700         0    -3.21276   0.84721  -6.22838  L
H-HC-0.032700         0    -4.68863   0.17449  -6.94342  L
H-HC-0.028500         0    -5.48294   2.50158  -7.43861  L
H-HC-0.028500         0    -4.1326    3.12634  -6.47737  L
H-H1-0.068700         0    -6.28009   1.23124  -5.45441  L
H-H1-0.068700         0    -6.22281   2.99047  -5.22636  L
H-H-0.345600          0    -3.80681   2.27091  -4.23728  L
H-H-0.447800          0    -6.77352   1.44062  -1.71694  L
H-H-0.447800          0    -7.02237   1.01178  -3.36314  L
H-H-0.447800          0    -4.87392   1.8049   -0.98254  L
H-H-0.447800          0    -3.53176   2.30162  -2.04831  L
N-N--0.415700         0    -2.35349   3.25286  -8.33446  L
C-CT--0.002400        -1   -1.28694   4.20959  -8.08314  L
C-C-0.597300          0    -1.75853   5.15639  -6.97303  L
O-O--0.567900         0    -2.90442   5.60388  -6.99823  L
C-CT--0.034300        0    -0.93265   4.96756  -9.37272  L
C-CA-0.011800         0    -0.39151   4.08676  -10.48863  L
C-CA--0.125600        0     0.97943   3.76897  -10.54692  L
C-CA--0.125600        0    -1.26684   3.55001  -11.45196  L
C-CA--0.170400        0     1.47323   2.9322   -11.56474  L
C-CA--0.170400        0    -0.77775   2.70335  -12.46228  L
C-CA--0.107200        0     0.59331   2.39998  -12.52367  L
H-H-0.271900          0    -3.28391   3.58221  -8.1278   L
H-H1-0.097800         0    -0.40231   3.688    -7.72885  L
H-HC-0.029500         0    -0.18853   5.72846  -9.13585  L
H-HC-0.029500         0    -1.82005   5.49266  -9.73059  L
H-HA-0.133000         0     1.6508    4.16177  -9.80162  L
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 H-HA-0.133000        0    -2.32383   3.76922  -11.40084  L
 H-HA-0.143000        0     2.5239    2.69283  -11.60249  L
 H-HA-0.143000        0    -1.46628   2.2759   -13.1775  L
 H-HA-0.129700        0     0.96081   1.74708  -13.30076  L
 N-N--0.516300        0    -0.91223   5.40242  -5.96987  L
 C-CT-0.038100        0    -1.31081   6.08159  -4.73422  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.52643   7.38697  -4.48368  L
 O-O--0.581900        0    -0.02644   7.63115  -3.37462  L
 C-CT--0.030300       0    -1.16804   5.11832  -3.55169  H
 C-C-0.799400         0    -1.9421    3.81116  -3.57458  H
 O-O2--0.801400       0    -2.24527   3.36918  -2.33583  H
 O-O2--0.801400       0    -2.26842   3.11737  -4.50409  H
 H-H-0.293600         0    -0.05482   4.8711   -5.93838  L
 H-H1-0.088000        0    -2.3625    6.36499  -4.7953   L
 H-HC--0.012200       0    -1.49091   5.65679  -2.65796  H
 H-HC--0.012200       0    -0.11314   4.83686  -3.45042  H
 N-N--0.516300        0    -0.45635   8.24896  -5.50115  L
 C-CT-0.038100        0     0.13619   9.5913   -5.45711  L
 C-C-0.536600         0    -0.83644   10.66272  -4.93447  L
 O-O--0.581900        0    -1.00973   11.74374  -5.49506  L
 C-CT--0.030300       0     0.80347   9.97165  -6.79793  L
 C-C-0.799400         0    -0.05781   9.81048  -8.06022  L
 O-O2--0.801400       0    -0.71693   8.75044  -8.1904   L
 O-O2--0.801400       0     0.04965   10.6892  -8.94437  L
 H-H-0.293600         0    -0.86155   8.0059   -6.40731  L
 H-H1-0.088000        0     0.93055   9.54751  -4.72266  L
 H-HC--0.012200       0     1.69112   9.35675  -6.91612  L
 H-HC--0.012200       0     1.16237   11.00069  -6.73229  L
 N-N--0.415700        0    -1.41232   10.40105  -3.75921  L
 C-CT--0.038900      -1    -2.21358   11.36391  -2.98019  L
 C-C-0.597300         0    -1.34289   12.56967  -2.4909   L
 O-O--0.567900        0    -1.90991   13.58265  -2.08525  L
 C-CT-0.365400        0    -2.91477   10.67528  -1.81793  L
 O-OH--0.676100       0    -2.05511   9.82299  -1.08415  L
 C-CT--0.243800      -1    -4.01196   9.83027  -2.44973  L
 H-H-0.271900         0    -1.20389   9.50521  -3.33505  L
 H-H1-0.100700        0    -2.97149   11.79656  -3.63284  L
 H-H1-0.004300        0    -3.35533   11.41316  -1.14883  L
 H-HC-0.064200        0    -4.70437   10.4711  -2.99387  L
 H-HC-0.064200        0    -4.54053   9.32818  -1.6461   L
 H-HC-0.064200        0    -3.59622   9.07707  -3.11895  L
 H-HO-0.410200        0    -1.89827   10.26991  -0.21676  L
 N-N--0.415700        0     0.01074   12.54019  -2.59117  L
 C-CT-0.014300       -1     0.93463   13.70367  -2.45851  L
 C-C-0.597300         0     1.89598   13.80967  -3.67327  L
 O-O--0.567900        0     3.0531    13.39477  -3.56626  L
 C-CT--0.204100       0     1.66004   13.69763  -1.10089  L
 C-C-0.713000         0     2.43622   14.99275  -0.87541  L
 O-O--0.593100        0     2.69794   15.79325  -1.76309  L
 N-N--0.919100        0     2.83031   15.27144   0.34102  L
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 H-H-0.271900         0     0.39022   11.69801  -3.00113  L
 H-H1-0.104800        0     0.32371   14.60511  -2.45124  L
 H-HC-0.079700        0     2.35121   12.85784  -1.05647  L
 H-HC-0.079700        0     0.92028   13.5893   -0.30634  L
 H-H-0.419600         0     3.31469   16.14307   0.43257  L
 H-H-0.419600         0     2.57956   14.68955   1.12909  L
 N-N--0.254800        0     1.47984   14.43913  -4.79712  L
 C-CT--0.026600       -1    2.23863   14.46665  -6.0593   L
 C-C-0.589600         0     3.60599   15.13652  -5.99793  L
 O-O--0.574800        0     4.4303    14.96067  -6.89203  L
 C-CT--0.007000       0     1.3063    15.07926  -7.10931  L
 C-CT-0.018900        0     0.29337   15.86766  -6.28447  L
 C-CT-0.019200        0     0.17375   15.05224  -4.99978  L
 H-H1-0.064100        0     2.41741   13.43187  -6.35278  L
 H-HC-0.025300        0     0.79115   14.2765   -7.64082  L
 H-HC-0.025300        0     1.83641   15.71842  -7.81663  L
 H-HC-0.021300        0    -0.66528   15.95542  -6.79667  L
 H-HC-0.021300        0     0.69907   16.85362  -6.0533   L
 H-H1-0.039100        0    -0.10131   15.7101   -4.17559  L
 H-H1-0.039100        0    -0.57841   14.27211  -5.12616  L
 N-N--0.415700        0     3.90307   15.89012  -4.94241  L
 C-CT--0.025200       -1    5.07901   16.7477   -4.90853  L
 C-C-0.597300         0     6.42056   16.10022  -4.57795  L
 O-O--0.567900        0     7.36995   16.77499  -4.18452  L
 H-H-0.271900         0     3.25454   15.8966   -4.16389  L
 H-H1-0.069800        0     4.90728   17.52497  -4.16436  L
 H-H1-0.069800        0     5.18545   17.24309  -5.87415  L
 N-N--0.347900        0     6.49757   14.79394  -4.78446  L
 C-CT--0.240000       -1    7.67231   13.92235  -4.70458  L
 C-C-0.734100         0     7.58752   12.83935  -5.81526  L
 O-O--0.589400        0     8.3627    11.88199  -5.781    L
 C-CT--0.009400       0     7.73265   13.31641  -3.27038  L
 C-CT-0.018700        0     6.5426    12.36666  -3.09028  L    H-HC
590   0.        0.
 C-CT--0.047900       0     6.20395   11.66511  -1.77135  H
 C-CT--0.014300       0     4.97373   10.88523  -2.24409  H
 N-N3--0.385400       0     4.23715   10.0264   -1.30406  H
 H-H-0.274700         0     5.61782   14.38764  -5.08154  L
 H-H1-0.142600        0     8.57326   14.51003  -4.88219  L
 H-HC-0.036200        0     7.68441   14.11478  -2.52794  L
 H-HC-0.036200        0     8.66355   12.76412  -3.13768  L
 H-HC-0.010300        0     6.7091    11.56768  -3.80024  L
 H-HC-0.010300        0     5.6507    12.92357  -3.37103  L
 H-HC-0.062100        0     5.96009   12.4045   -1.0073   H
 H-HC-0.062100        0     7.02242   11.02437  -1.44726  H
 H-HP-0.113500        0     5.25528   10.22102  -3.06722  H
 H-HP-0.113500        0     4.26042   11.6023   -2.67685  H
 H-H-0.340000         0     3.37227   9.81461   -1.81499  H
 H-H-0.340000         0     3.96176   10.57738  -0.4851   H
 H-H-0.340000         0     4.92623   8.67677   -0.733    H
 N-N--0.516300        0     6.61782   12.92789  -6.74089  L
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C-CT-0.039700        -1    6.11755   11.82076  -7.58383  L
C-C-0.536600         0     6.29327   12.13595  -9.09913  L
O-O--0.581900        0     6.15165   13.28194  -9.51888  L
C-CT-0.056000        0     4.70279   11.36296  -7.1471   L
C-CT-0.013600        0     4.7397    11.06587  -5.63432  L
C-C-0.805400         0     3.75697   10.06635  -5.00394  L
O-O2--0.818800       0     2.92701   10.48288  -4.1666   L
O-O2--0.818800       0     4.06072   8.85675  -5.08357  L
H-H-0.293600         0     6.06896   13.77867  -6.81     L
H-H1-0.110500        0     6.76438   10.9617  -7.4065   L
H-HC--0.017300       0     4.45365   10.46745  -7.70317  L
H-HC--0.017300       0     3.96583   12.13477  -7.36361  L
H-HC--0.042500       0     4.65793   12.01991  -5.11853  L
H-HC--0.042500       0     5.72629   10.65447  -5.42786  L
N-N--0.415700        0     6.72033   11.14943  -9.91627  L
C-CT--0.149000       -1    7.15878   11.32433  -11.32085  L
H-H-0.271900         0     6.78337   10.22701  -9.51314  L
H-H1-0.097600        0     7.96665   12.05656  -11.3633  L
H-H1-0.097600        0     6.32099   11.69573  -11.91465  L
H-H1-0.097600        0     7.50043   10.37375  -11.73112  L
C-CT--0.366200       0     10.30606   1.40833  -12.20086  L
C-C-0.597200         0     9.15612   0.91636  -11.35562  L
O-O--0.567900        0     9.35928   0.59106  -10.19103  L
H-HC-0.112300        0     10.86792   2.13594  -11.61854  L
H-HC-0.112300        0     9.94705   1.87397  -13.11592  L
H-HC-0.112300        0     10.94788   0.5615   -12.43616  L
N-N--0.415700        0     7.95579   0.88191  -11.94158  L
C-CT--0.059700       -1    6.71955   0.39188  -11.30758  L
C-C-0.597300         0     5.9429   -0.50836  -12.28701  L
O-O--0.567900        0     6.12623  -1.72132  -12.26084  L
C-CT-0.130300        0     5.87959   1.54395  -10.685   L
C-CT--0.043000       0     6.70643   2.34226  -9.64426  L
C-CT--0.320400       0     4.60541   0.99185  -10.01175  L
C-CT--0.066000       0     5.98951   3.55171  -9.0365   L
H-H-0.271900         0     7.9218    1.15224  -12.91021  L
H-H1-0.086900        0     7.01144  -0.26146  -10.48579  L
H-HC-0.018700        0     5.5808    2.22762  -11.48142  L
H-HC-0.023600        0     7.60167   2.73612  -10.12252  L
H-HC-0.023600        0     7.01857   1.6759   -8.83825  L
H-HC-0.088200        0     4.02178   0.37678  -10.69544  L
H-HC-0.088200        0     3.96266   1.81268  -9.69672  L
H-HC-0.088200        0     4.8673    0.39435  -9.13871  L
H-HC-0.018600        0     5.15754   3.23339  -8.41139  L
H-HC-0.018600        0     5.62347   4.20346  -9.83049  L
H-HC-0.018600        0     6.69228   4.10925  -8.41614  L
N-N--0.415700        0     5.10407   0.06237  -13.16496  L
C-CT--0.149000       -1    4.28063  -0.68155  -14.12252  L
H-H-0.271900         0     4.99265   1.0624   -13.11124  L
H-H1-0.097600        0     3.77051  -1.5013   -13.61138  L
H-H1-0.097600        0     4.91228  -1.10188  -14.90679  L
H-H1-0.097600        0     3.53321  -0.02474  -14.57038  L
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C-CT--0.366200       -1   -5.06516   16.94133  -3.23542  L
C-C-0.597200         0    -5.63502   16.17498  -2.05469  L
O-O--0.567900        0    -5.46998   16.62152  -0.92273  L
H-HC-0.112300        0    -5.87556   17.34208  -3.83913  L
H-HC-0.112300        0    -4.4378    16.27369  -3.82469  L
H-HC-0.112300        0    -4.45268   17.75774  -2.85687  L
N-N--0.254800        0    -6.36485   15.07358  -2.29597  L
C-CT--0.026600       -1   -7.05186   14.32732  -1.24795  L
C-C-0.589600         0    -6.19966   13.22518  -0.62263  L
O-O--0.574800        0    -5.68602   12.33143  -1.29332  L
C-CT--0.007000       0    -8.26247   13.72195  -1.96852  L
C-CT-0.018900        0    -7.73626   13.43663  -3.37791  L
C-CT-0.019200        0    -6.74041   14.57343  -3.61429  L
H-H1-0.064100        0    -7.40464   15.00489  -0.46971  L
H-HC-0.025300        0    -9.05921   14.4652  -2.02372  L
H-HC-0.025300        0    -8.62696   12.81798  -1.48063  L
H-HC-0.021300        0    -8.53921   13.44561  -4.11533  L
H-HC-0.021300        0    -7.21515   12.47929  -3.40185  L
H-H1-0.039100        0    -5.86729   14.20145  -4.15272  L
H-H1-0.039100        0    -7.22591   15.36613  -4.18431  L
N-N--0.415700        0    -6.12644   13.27992   0.69975  L
C-CT--0.023700       -1   -5.2815    12.4434   1.53918  L
C-C-0.597300         0    -5.47275   10.91708   1.4105   L
O-O--0.567900        0    -6.56184   10.43537   1.08565  L
C-CT-0.034200        0    -5.53645   12.81733   3.01343  L
C-CT-0.001800        0    -5.10432   14.23929   3.40268  L
S-S--0.273700        0    -3.32097   14.51146   3.60633  L
C-CT--0.053600       -1   -3.00424   13.55115   5.11582  L
H-H-0.271900         0    -6.58697   14.05862   1.13754  L
H-H1-0.088000        0    -4.23727   12.66055   1.30133  L
H-HC-0.024100        0    -5.0204    12.11041   3.66314  L
H-HC-0.024100        0    -6.60447   12.7159   3.21321  L
H-H1-0.044000        0    -5.58354   14.48843   4.34959  L
H-H1-0.044000        0    -5.47422   14.94219   2.65644  L
H-H1-0.068400        0    -3.19381   12.4941   4.92816  L
H-H1-0.068400        0    -3.64663   13.90008   5.92337  L
H-H1-0.068400        0    -1.96027   13.66235   5.40673  L
N-N--0.415700        0    -4.41753   10.16703   1.75957  L
C-CT--0.001400       -1   -4.28218   8.71407   1.62049  L
C-C-0.597300         0    -5.528     7.84962   1.92577  L
O-O--0.567900        0    -6.11518   7.34221   0.97541  L
C-CT--0.015200       0    -3.01453   8.18399   2.31058  L
C-CA--0.001100       0    -2.95552   6.68173   2.53404  L
C-CA--0.190600       0    -3.28403   5.77305   1.5078   L
C-CA--0.190600       0    -2.67008   6.19979   3.82136  L
C-CA--0.234100       0    -3.3503    4.39309   1.78876  L
C-CA--0.234100       0    -2.7819    4.83106   4.11246  L
C-C-0.322600         0    -3.12663   3.92229   3.09838  L
O-OH--0.557900       0    -3.26883   2.60152   3.37551  L
H-H-0.271900         0    -3.54681   10.65913   1.94732  L
H-H1-0.087600        0    -4.10795   8.55346   0.55673  L
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H-HC-0.029500        0    -2.92464   8.68146   3.27599  L
H-HC-0.029500        0    -2.15435   8.44781   1.70114  L
H-HA-0.169900        0    -3.56404   6.14531   0.52999  L
H-HA-0.169900        0    -2.44603   6.89459   4.61737  L
H-HA-0.165600        0    -3.65389   3.68312   1.03661  L
H-HA-0.165600        0    -2.67558   4.49286   5.13021  L
H-HO-0.399200        0    -3.57588   2.48222   4.29557  L
N-N--0.516300        0    -5.88614   7.56153   3.18503  L
C-CT-0.038100       -1    -6.83192   6.48081   3.56286  L
C-C-0.536600         0    -8.23449   6.68545   2.98813  L
O-O--0.581900        0    -8.88494   5.71819   2.60099  L
C-CT--0.030300       0    -6.90642   6.33067   5.09428  L
C-C-0.799400         0    -5.63624   5.72015   5.69887  L
O-O2--0.801400       0    -5.50984   4.47178   5.65168  L
O-O2--0.801400       0    -4.79006   6.49764   6.20571  L
H-H-0.293600         0    -5.39058   8.04661   3.92898  L
H-H1-0.088000        0    -6.45074   5.53936   3.17319  L
H-HC--0.012200       0    -7.74249   5.67462   5.33954  L
H-HC--0.012200       0    -7.11353   7.3003    5.54938  L
N-N--0.415700        0    -8.68614   7.93887   2.89704  L
C-CT--0.002400       0    -9.87839   8.32512   2.14139  L
C-C-0.597300         0    -9.7753    7.87553   0.67569  L
O-O--0.567900        0    -10.62644   7.13377   0.18502  L
C-CT--0.034300       0    -10.08611   9.8432    2.25517  L
C-CA-0.011800        0    -11.14058   10.38236   1.30631  L
C-CA--0.125600       0    -12.5076   10.2018   1.58855  L
C-CA--0.125600       0    -10.75208   11.00721   0.10539  L
C-CA--0.170400       0    -13.48101   10.64844   0.67631  L
C-CA--0.170400       0    -11.72451   11.45139  -0.80738  L
C-CA--0.107200       0    -13.0896   11.27268  -0.52172  L
H-H-0.271900         0    -8.04444   8.65487   3.20698  L
H-H1-0.097800        0    -10.74602   7.82263   2.57033  L
H-HC-0.029500        0    -9.14181   10.35026   2.05026  L
H-HC-0.029500        0    -10.37173   10.08474   3.27971  L
H-HA-0.133000        0    -12.80999   9.70087   2.49708  L
H-HA-0.133000        0    -9.70248   11.11956  -0.13237  L
H-HA-0.143000        0    -14.52913   10.49533   0.8892   L
H-HA-0.143000        0    -11.41645   11.91102  -1.73577  L
H-HA-0.129700        0    -13.83646   11.60194  -1.22984  L
N-N--0.415700        0    -8.7377    8.3171   -0.0326   L
C-CT--0.038900      -1    -8.54772   8.01592  -1.45561  L
C-C-0.597300         0    -8.37182   6.53613  -1.74724  L
O-O--0.567900        0    -9.01227   5.98592  -2.63979  L
C-CT-0.365400        0    -7.39963   8.85067  -2.03344  L
O-OH--0.676100       0    -7.66653   10.21915  -1.80961  L
C-CT--0.243800       0    -7.25088   8.6755   -3.54549  L
H-H-0.271900         0    -8.06095   8.92753   0.41524  L
H-H1-0.100700        0    -9.45339   8.32535  -1.97695  L
H-H1-0.004300        0    -6.47809   8.56817  -1.53098  L
H-HC-0.064200        0    -8.20271   8.87838  -4.03668  L
H-HC-0.064200        0    -6.93238   7.65976  -3.77907  L
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H-HC-0.064200        0    -6.50499   9.36875  -3.93032  L
H-HO-0.410200        0    -6.8307    10.66591  -1.59903  L
N-N--0.415700        0    -7.53205   5.88914  -0.95102  L
C-CT--0.058100       -1   -7.39431   4.4473   -0.81203  L
C-C-0.597300         0    -8.74231   3.753    -0.67868  L
O-O--0.567900        0    -9.05649   2.89741  -1.5059   L
C-CT--0.007400       0    -6.46292   4.2232    0.37975  L
C-CC-0.186800        0    -6.40018   2.82904   0.92438  L
N-NB--0.543200       0    -6.51707   1.66502   0.17667  L
C-CW--0.220700       0    -6.26506   2.50647   2.23895  L
C-CR-0.163500        0    -6.49388   0.65345   1.04872  L
N-NA--0.279500       0    -6.32231   1.13467   2.28955  L
H-H-0.271900         0    -7.07664   6.46702  -0.25125  L
H-H1-0.136000        0    -6.92395   4.04383  -1.70854  L
H-HC-0.036700        0    -6.7904    4.86133   1.19295  L
H-HC-0.036700        0    -5.46648   4.53643   0.08047  L
H-H4-0.186200        0    -6.16554   3.19006   3.07411  L
H-H-0.333900         0    -6.29442   0.55054   3.12355  L
H-H5-0.143500        0    -6.61707  -0.39008   0.78433  L
N-N--0.415700        0    -9.5438    4.13099   0.32273  L
C-CT-0.021300        -1   -10.8414   3.50754   0.53492  L
C-C-0.597300         0    -11.75486   3.54917  -0.66826  L
O-O--0.567900        0    -12.36662   2.54583  -1.03191  L
C-CT--0.123100       0    -11.49739   3.90804   1.87423  L
S-SH--0.311900       0    -12.58984   5.3561    1.78927  L
H-H-0.271900         0    -9.2353    4.84729   0.97214  L
H-H1-0.112400        0    -10.62062   2.44469   0.64463  L
H-H1-0.111200        0    -10.72604   4.08032   2.62404  L
H-H1-0.111200        0    -12.097    3.06451   2.22004  L
H-HS-0.193300        0    -11.68323   6.19535   1.27025  L
N-N--0.415700        0    -11.79726   4.70937  -1.30182  L
C-CT--0.059700       -1   -12.61165   4.92721  -2.46941  L
C-C-0.597300         0    -12.11589   4.21364  -3.72821  L
O-O--0.567900        0    -12.9264   3.58832  -4.41045  L
C-CT-0.130300        0    -12.84061   6.45181  -2.65459  L
C-CT--0.043000       0    -14.17643   6.89934  -2.01035  L
C-CT--0.320400       -1   -12.74698   6.95159  -4.10194  L
C-CT--0.066000       -1   -15.46532   6.49368  -2.75608  L
H-H-0.271900         0    -11.25642   5.47409  -0.91191  L
H-H1-0.086900        0    -13.58192   4.47608  -2.26424  L
H-HC-0.018700        0    -12.04757   6.97754  -2.11904  L
H-HC-0.023600        0    -14.16751   7.9869   -1.92525  L
H-HC-0.023600        0    -14.22232   6.49933  -0.99619  L
H-HC-0.088200        0    -11.727    6.84034  -4.47142  L
H-HC-0.088200        0    -12.99997   8.01115  -4.14124  L
H-HC-0.088200        0    -13.42828   6.39749  -4.74922  L
H-HC-0.018600        0    -16.33052   6.80399  -2.16999  L
H-HC-0.018600        0    -15.50321   5.41308  -2.89298  L
H-HC-0.018600        0    -15.51114   6.98369  -3.72844  L
N-N--0.415700        0    -10.82307   4.30173  -4.0572   L
C-CT--0.024900       -1   -10.24933   3.56819  -5.19084  L
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C-C-0.597300          0    -10.51425   2.05798  -5.01367  L
O-O--0.567900         0    -10.92592   1.41848  -5.97395  L
C-CT-0.211700         0    -8.75934    3.83638  -5.33563  L
O-OH--0.654600        0    -8.30681    3.27957  -6.55671  L
H-H-0.271900          0    -10.21339    4.84223  -3.45129  L
H-H1-0.084300         0    -10.74983    3.8943   -6.10323  L
H-H1-0.035200         0    -8.22912    3.39101  -4.49267  L
H-H1-0.035200         0    -8.57675    4.91199  -5.34333  L
H-HO-0.427500         0    -8.85222    2.51366  -6.78601  L
N-N--0.516300         0    -10.31084    1.48631  -3.81473  L
C-CT-0.038100         -1   -10.56313    0.05877  -3.52704  L
C-C-0.536600          0    -12.04218  -0.34404  -3.63662  L
O-O--0.581900         0    -12.37444  -1.30279  -4.339    L
C-CT--0.030300        0    -9.9569    -0.36193  -2.17674  L
C-C-0.799400          0    -8.49012   -0.76929  -2.3194   L
O-O2--0.801400        0    -7.90809   -0.57672  -3.41063  L
O-O2--0.801400        0    -7.90301   -1.28234  -1.33999  L
H-H-0.293600          0    -9.96435    2.06647  -3.05703  L
H-H1-0.088000         0    -10.07524  -0.51446  -4.31374  L
H-HC--0.012200        0    -10.50513  -1.22014  -1.78742  L
H-HC--0.012200        0    -10.05593    0.44528  -1.45038  L
N-N--0.415700         0    -12.9324    0.38803  -2.96274  L
C-CT-0.033700         -1   -14.38616    0.2599   -3.08497  L
C-C-0.597300          0    -14.85671    0.26816  -4.55119  L
O-O--0.567900         0    -15.68307  -0.55266  -4.94513  L
C-CT--0.182500        -1   -14.99785    1.42353  -2.36497  L
H-H-0.271900          0    -12.57762    1.15338  -2.39802  L
H-H1-0.082300         0    -14.71148  -0.67424  -2.62625  L
H-HC-0.060300         0    -14.7343    1.38233  -1.30763  L
H-HC-0.060300         0    -16.08431    1.3744   -2.44951  L
H-HC-0.060300         0    -14.65123    2.36777  -2.7842   L
N-N--0.415700         0    -14.36432    1.23751  -5.32924  L
C-CT--0.025200        -1   -14.73708    1.48111  -6.71903  L
C-C-0.597300          0    -14.2453    0.4163   -7.69567  L
O-O--0.567900         0    -14.98461    0.01043  -8.58714  L
H-H-0.271900          0    -13.7035    1.87946  -4.90316  L
H-H1-0.069800         0    -14.32753    2.44051  -7.03256  L
H-H1-0.069800         0    -15.82335    1.52899  -6.79315  L
N-N--0.516300         0    -12.99424  -0.00891  -7.53618  L
C-CT-0.039700         -1   -12.35956  -1.10333  -8.27562  L
C-C-0.536600          0    -13.09384  -2.44577  -8.09752  L
O-O--0.581900         0    -13.23393  -3.20705  -9.05133  L
C-CT-0.056000         0    -10.89735  -1.16249  -7.80631  L
C-CT-0.013600         0    -10.02042  -2.25455  -8.42786  L
C-C-0.805400          0    -9.58326   -1.96792  -9.86634  L
O-O2--0.818800        0    -9.57924   -2.91288  -10.6866  L
O-O2--0.818800        0    -9.09636   -0.84665  -10.12772  L
H-H-0.293600          0    -12.43372    0.43459  -6.81506  L
H-H1-0.110500         0    -12.37023  -0.87107  -9.3415   L
H-HC--0.017300        0    -10.91088  -1.31633  -6.73037  L
H-HC--0.017300        0    -10.42715  -0.1955   -7.98597  L
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H-HC--0.042500       0    -10.54612  -3.2037   -8.36693  L
H-HC--0.042500       0    -9.11477  -2.3438   -7.82512  L
N-N--0.415700        0    -13.54941  -2.74522  -6.87599  L
C-CT--0.025200       -1   -14.25257  -3.98797  -6.52252  L
C-C-0.597300         0    -13.50788  -4.84324  -5.51317  L
O-O--0.567900        0    -13.85351  -6.0156   -5.34831  L
H-H-0.271900         0    -13.42668  -2.03029  -6.16822  L
H-H1-0.069800        0    -14.42299  -4.59192  -7.4142   L
H-H1-0.069800        0    -15.22204  -3.73137  -6.09736  L
N-N--0.415700        0    -12.49708  -4.28181  -4.83266  L
C-CT--0.059700       -1   -11.76657  -4.98363  -3.77657  L
C-C-0.597300         0    -12.78911  -5.52272  -2.77117  L
O-O--0.567900        0    -13.71838  -4.82082  -2.37746  L
C-CT-0.130300        0    -10.7046  -4.0847   -3.0892   L
C-CT--0.043000       0    -9.38052  -4.02644  -3.87015  L
C-CT--0.320400       0    -10.28861  -4.57858  -1.68607  L
C-CT--0.066000       0    -9.45529  -3.45881  -5.28067  L
H-H-0.271900         0    -12.33915  -3.28883  -4.96653  L
H-H1-0.086900        0    -11.26334  -5.8272   -4.23064  L
H-HC-0.018700        0    -11.10871  -3.08131  -2.9798   L
H-HC-0.023600        0    -8.97864  -5.02896  -3.932    L
H-HC-0.023600        0    -8.67566  -3.41609  -3.3092   L
H-HC-0.088200        0    -9.53909  -3.90673  -1.26328  L
H-HC-0.088200        0    -9.87582  -5.5866   -1.74367  L
H-HC-0.088200        0    -11.13914  -4.57027  -1.01302  L
H-HC-0.018600        0    -8.45548  -3.42752  -5.711    L
H-HC-0.018600        0    -9.85138  -2.45095  -5.23359  L
H-HC-0.018600        0    -10.08783  -4.08044  -5.91035  L
N-N--0.415700        0    -12.6069  -6.77308  -2.34457  L
C-CT--0.025200       -1   -13.46387  -7.4109   -1.33722  L
C-C-0.597300         0    -12.91352  -7.34086   0.07033  L
O-O--0.567900        0    -13.64282  -7.13339   1.03804  L
H-H-0.271900         0    -11.86233  -7.28265  -2.80313  L
H-H1-0.069800        0    -13.59626  -8.45965  -1.5983   L
H-H1-0.069800        0    -14.45002  -6.94395  -1.33996  L
N-N--0.415700        0    -11.60562  -7.53437   0.16668  L
C-CT--0.058100       -1   -10.85454  -7.52006   1.4035   L
C-C-0.597300         0    -9.47664  -6.87883   1.13395  L
O-O--0.567900        0    -8.7405   -7.36721   0.2777   L
C-CT--0.007400       0    -10.70697  -8.96138   1.92109  L
C-CC-0.186800        0    -12.00507  -9.54678   2.42918  L
N-NB--0.543200       0    -12.60984  -9.25806   3.65585  L
C-CW--0.220700       0    -12.81781  -10.38331   1.72151  L
C-CR-0.163500        0    -13.77888  -9.91323   3.65189  L
N-NA--0.279500       0    -13.92973  -10.60166   2.50636  L
H-H-0.271900         0    -11.08284  -7.65752  -0.68872  L
H-H1-0.136000        0    -11.37549  -6.92846   2.15798  L
H-HC-0.036700        0    -9.97209  -8.98363   2.72332  L
H-HC-0.036700        0    -10.3211  -9.59351   1.11982  L
H-H4-0.186200        0    -12.62867  -10.7514   0.72337  L
H-H-0.333900         0    -14.74476  -11.14194   2.25702  L
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H-H5-0.143500        0    -14.50174  -9.87881   4.45682  L
N-N--0.415700        0    -9.1276   -5.77327   1.80439  L
C-CT--0.024900       -1   -7.86643  -5.04108   1.5711   L
C-C-0.597300         0    -6.67585  -5.66906   2.29711  L
O-O--0.567900        0    -6.72057  -5.93626   3.49764  L
C-CT-0.211700        0    -7.99465  -3.54698   1.89708  L
O-OH--0.654600       0    -6.7179   -2.91969   1.87133  L
H-H-0.271900         0    -9.74188  -5.47665   2.55483  L
H-H1-0.084300        0    -7.65283  -5.09142   0.50269  L
H-H1-0.035200        0    -8.44418  -3.42936   2.8763   L
H-H1-0.035200        0    -8.64674  -3.0711    1.16233  L
H-HO-0.427500        0    -6.73662  -2.15519   2.47732  L
N-N--0.415700        0    -5.5828   -5.8714    1.55887  L
C-CT--0.051800       -1   -4.28216  -6.26875   2.09329  L
C-C-0.597300         0    -3.40397  -5.05064   2.3196   L
O-O--0.567900        0    -3.1866   -4.27228   1.39199  L
C-CT--0.110200       0    -3.59329  -7.25298   1.12354  L
C-CT-0.353100        0    -4.10361  -8.70691   1.14659  L
C-CT--0.412100       0    -5.48429  -8.88485   0.51384  L
C-CT--0.412100       0    -3.12453  -9.58924   0.36522  L
H-H-0.271900         0    -5.65772  -5.66409   0.57479  L
H-H1-0.092200        0    -4.41964  -6.77152   3.05379  L
H-HC-0.045700        0    -2.53963  -7.2833    1.39139  L
H-HC-0.045700        0    -3.65331  -6.86789   0.10841  L
H-HC--0.036100       0    -4.13444  -9.05994   2.17766  L
H-HC-0.100000        0    -5.4948   -8.47516  -0.49682  L
H-HC-0.100000        0    -6.24157  -8.38324   1.11393  L
H-HC-0.100000        0    -5.74298  -9.94185   0.47505  L
H-HC-0.100000        0    -2.13144  -9.52383   0.80906  L
H-HC-0.100000        0    -3.07982  -9.26329  -0.67456  L
H-HC-0.100000        0    -3.4565   -10.62668   0.39934  L
N-N--0.415700        0    -2.85946  -4.92414   3.52262  L
C-CT-0.021300        -1   -1.91397  -3.86735   3.85113  L
C-C-0.597300         0    -0.77883  -4.37754   4.75639  L
O-O--0.567900        0    -0.78788  -5.53452   5.17974  L
C-CT--0.123100       0    -2.71269  -2.71644   4.47376  L
S-SH--0.311900       0    -1.77621  -1.16761   4.40187  L
H-H-0.271900         0    -3.11253  -5.58324   4.25112  L
H-H1-0.112400        0    -1.44689  -3.4971    2.93516  L
H-H1-0.111200        0    -2.97291  -2.9527    5.5074   L
H-H1-0.111200        0    -3.63115  -2.57485   3.90348  L
H-HS-0.193300        0    -2.66374  -0.42824   5.08197  L
N-N--0.415700        0     0.21041  -3.54183   5.0744   L
C-CT--0.038900       -1    1.3155   -3.91043   5.97259  L
C-C-0.597300         0     1.44032  -3.00542   7.17517  L
O-O--0.567900        0     0.77544  -1.98435   7.3247   L
C-CT-0.365400        0     2.67493  -4.06267   5.2617   L
O-OH--0.676100       0     3.11627  -2.86836   4.65527  L
C-CT--0.243800       0     2.65501  -5.18788   4.23062  L
H-H-0.271900         0     0.13175  -2.587     4.74325  L
H-H1-0.100700        0     1.09444  -4.89138   6.393    L
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H-H1-0.004300        0     3.42571  -4.34541   5.99964  L
H-HC-0.064200        0     1.96056  -4.9609    3.42358  L
H-HC-0.064200        0     2.34186  -6.11727   4.70745  L
H-HC-0.064200        0     3.65309  -5.31881   3.82256  L
H-HO-0.410200        0     3.46794  -2.27444   5.3588   L
N-N--0.415700        0     2.27811  -3.4835    8.08663  L
C-CT--0.051800       -1    2.19107  -3.18196   9.49278  L
C-C-0.597300         0     2.27513  -1.68158   9.86697  L
O-O--0.567900        0     1.71261  -1.28866   10.87953  L
C-CT--0.110200       0     3.19669  -4.04756   10.2207  L
C-CT-0.353100        0     2.8937   -4.11842   11.71903  L
C-CT--0.412100       0     1.55404  -4.76946   12.07513  L
C-CT--0.412100       -1    3.98899  -5.00634   12.24798  L
H-H-0.271900         0     2.74139  -4.34011   7.84163  L
H-H1-0.092200        0     1.18925  -3.4906    9.79245  L
H-HC-0.045700        0     4.19318  -3.63312   10.05915  L
H-HC-0.045700        0     3.1596   -5.05793   9.80829  L
H-HC--0.036100       0     2.97778  -3.13933   12.18714  L
H-HC-0.100000        0     1.43949  -5.72758   11.56967  L
H-HC-0.100000        0     0.73205  -4.1128    11.797   L
H-HC-0.100000        0     1.48965  -4.91644   13.15421  L
H-HC-0.100000        0     3.8793   -5.09241   13.32983  L
H-HC-0.100000        0     4.96505  -4.56633   12.04572  L
H-HC-0.100000        0     3.92641  -6.00343   11.81231  L
N-N--0.516300        0     2.94692  -0.83946   9.07728  L
C-CT-0.039700        -1    3.07274   0.61629   9.31166  L
C-C-0.536600         0     1.8177    1.45943   8.99195  L
O-O--0.581900        0     1.88258   2.69068   9.01215  L
C-CT-0.056000        0     4.31738   1.12908   8.55099  L
C-CT-0.013600        0     4.30219   0.96805   7.01662  L
C-C-0.805400         0     4.93491  -0.3394    6.52585  L
O-O2--0.818800       0     4.29311  -1.41688   6.57622  L
O-O2--0.818800       0     6.12682  -0.328     6.12119  L
H-H-0.293600         0     3.2917   -1.21115   8.19651  L
H-H1-0.110500        0     3.25358   0.77499   10.37571  L
H-HC--0.017300       0     5.20324   0.62827   8.94562  L
H-HC--0.017300       0     4.43754   2.18923   8.77685  L
H-HC--0.042500       0     4.89435   1.78192   6.59845  L
H-HC--0.042500       0     3.28543   1.06284   6.63756  L
N-N--0.415700        0     0.68009   0.80725   8.73871  L
C-CT--0.002400       -1   -0.63589   1.42644   8.53893  L
C-C-0.597300         0    -1.77137   0.78371   9.35053  L
O-O--0.567900        0    -2.94985   1.09383   9.15988  L
C-CT--0.034300       0    -1.01729   1.28219   7.05763  L
C-CA-0.011800        0    -0.08217   1.86003   6.01796  L
C-CA--0.125600       0    -0.20209   3.21057   5.65071  L
C-CA--0.125600       0     0.80433   1.02117   5.31872  L
C-CA--0.170400       0     0.50645   3.70486   4.54418  L
C-CA--0.170400       0     1.55026   1.52694   4.24168  L
C-CA--0.107200       0     1.38604   2.8642    3.84081  L
H-H-0.271900         0     0.74667  -0.19694   8.63347  L
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H-H1-0.097800        0    -0.59281   2.48503   8.79446  L
H-HC-0.029500        0    -1.98745   1.75317   6.90422  L
H-HC-0.029500        0    -1.14931   0.21997   6.8497   L
H-HA-0.133000        0    -0.87099   3.85932   6.19638  L
H-HA-0.133000        0     0.88946  -0.02048   5.59044  L
H-HA-0.143000        0     0.36244   4.73159   4.24148  L
H-HA-0.143000        0     2.21951   0.87478   3.70124  L
H-HA-0.129700        0     1.93553   3.24284   2.99017  L
N-N--0.415700        0    -1.40917  -0.12468   10.24508  L
C-CT--0.003100      -1    -2.27426  -0.99348   11.02542  L
C-C-0.597300         0    -3.51811  -0.29091   11.62902  L
O-O--0.567900        0    -4.65816  -0.63409   11.33194  L
C-CT--0.003600       0    -1.35691  -1.57713   12.12057  L
C-CT--0.064500       0    -2.01746  -2.31281   13.29949  L
C-C-0.695100         0    -1.09276  -2.34005   14.51553  L
O-O--0.608600        0    -0.63986  -3.38304   14.95944  L
N-N--0.940700        0    -0.7773   -1.20968   15.11646  L
H-H-0.271900         0    -0.41219  -0.19968   10.40692  L
H-H1-0.085000        0    -2.64867  -1.79783   10.40686  L
H-HC-0.017100        0    -0.77586  -0.74963   12.53077  L
H-HC-0.017100        0    -0.64909  -2.25776   11.64966  L
H-HC-0.035200        0    -2.25861  -3.33218   12.99703  L
H-HC-0.035200        0    -2.93915  -1.82556   13.60922  L
H-H-0.425100         0    -0.14454  -1.3183    15.88247  L
H-H-0.425100         0    -1.04244  -0.28081   14.7778  L
N-N--0.516300        0    -3.30367   0.63466   12.55802  L
C-CT-0.038100       -1    -4.28257   1.5025    13.2509  L
C-C-0.536600         0    -4.85692   2.57102   12.318   L
O-O--0.581900        0    -6.04966   2.8694    12.37497  L
C-CT--0.030300       0    -3.56845   2.14565   14.45738  L
C-C-0.799400         0    -2.10669   2.462     14.12402  L
O-O2--0.801400       0    -1.85844   3.46772   13.42392  L
O-O2--0.801400       0    -1.26171   1.55996   14.34893  L
H-H-0.293600         0    -2.32513   0.7944    12.77429  L
H-H1-0.088000        0    -5.11834   0.90294   13.61242  L
H-HC--0.012200       0    -3.59259   1.44043   15.29019  L
H-HC--0.012200       0    -4.09249   3.0516    14.76659  L
N-N--0.415700        0    -4.01119   3.11598   11.43901  L
C-CT-0.014300       -1    -4.36345   4.12505   10.44408  L
C-C-0.597300         0    -5.61235   3.78101   9.6335   L
O-O--0.567900        0    -6.40792   4.66013   9.30347  L
C-CT--0.204100       0    -3.16044   4.43339   9.53236  L
C-C-0.713000         0    -2.16884   5.43808   10.09218  L
O-O--0.593100        0    -1.76476   6.36055   9.40519  L
N-N--0.919100        0    -1.69921   5.31477   11.31245  L
H-H-0.271900         0    -3.04984   2.81607   11.51352  L
H-H1-0.104800        0    -4.61827   5.04371   10.97608  L
H-HC-0.079700        0    -3.54069   4.85996   8.60171  L
H-HC-0.079700        0    -2.62657   3.52791   9.27494  L
H-H-0.419600         0    -1.0594    6.04344   11.56014  L
H-H-0.419600         0    -1.95522   4.5955    11.99226  L
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N-N--0.347900        0    -5.80195   2.49147   9.34915  L
C-CT--0.263700       -1   -6.94568   1.98285   8.60004  L
C-C-0.734100         0    -8.34366   2.29433   9.1525   L
O-O--0.589400        0    -9.32973   2.08194   8.44905  L
C-CT--0.000700       0    -6.76247   0.47955   8.32421  L
C-CT-0.039000        0    -7.35196  -0.40309   9.42876  L
C-CT-0.048600        0    -6.93907  -1.86438   9.27116  L
N-N2--0.529500       0    -7.6151   -2.66261   10.30019  L
C-CA-0.807600        0    -7.10985  -3.03385   11.45142  L
N-N2--0.862700       0    -5.83878  -3.11918   11.68548  L
N-N2--0.862700       0    -7.90048  -3.27412   12.44773  L
H-H-0.274700         0    -5.07243   1.85388   9.65032  L
H-H1-0.156000        0    -6.91538   2.48497   7.63088  L
H-HC-0.032700        0    -5.69892   0.26029   8.21417  L
H-HC-0.032700        0    -7.26189   0.23197   7.386    L
H-HC-0.028500        0    -8.44094  -0.34784   9.39521  L
H-HC-0.028500        0    -7.01607  -0.04083   10.40078  L
H-H1-0.068700        0    -5.85726  -1.92873   9.36616  L
H-H1-0.068700        0    -7.22066  -2.23005   8.28685  L
H-H-0.345600         0    -8.62318  -2.73061   10.24364  L
H-H-0.447800         0    -5.46998  -2.17797   11.7656  L
H-H-0.447800         0    -5.35397  -3.48673   10.85681  L
H-H-0.447800         0    -7.47276  -3.50265   13.31991  L
H-H-0.447800         0    -8.8753   -2.99559   12.34309  L
N-N--0.415700        0    -8.46449   2.76435   10.39049  L
C-CT--0.149000       -1   -9.75082   3.10638   10.97095  L
H-H-0.271900         0    -7.61137   2.90406   10.92119  L
H-H1-0.097600        0    -10.33077   3.71398   10.27522  L
H-H1-0.097600        0    -9.59803   3.66448   11.89531  L
H-H1-0.097600        0    -10.30157   2.19003   11.19299  L
C-CT--0.366200       -1   -9.95663   6.30611   8.76062  L
C-C-0.597200         0    -10.67058   5.55821   7.6593   L
O-O--0.567900        0    -11.85215   5.80225   7.4535   L
H-HC-0.112300        0    -9.14177   5.70202   9.16032  L
H-HC-0.112300        0    -10.66552   6.53808   9.55237  L
H-HC-0.112300        0    -9.5526    7.22911   8.34883  L
N-N--0.415700        0    -9.97847   4.63942   6.98205  L
C-CT--0.001400       -1   -10.50133   3.78979   5.89165  L
C-C-0.597300         0    -11.83415   3.09038   6.19654  L
O-O--0.567900        0    -12.70786   2.94737   5.3381   L
C-CT--0.015200       0    -9.36474   2.88947   5.35387  L
C-CA--0.001100       0    -9.75575   1.65262   4.56582  L
C-CA--0.190600       0    -10.36216   0.56654   5.22563  L
C-CA--0.190600       0    -9.4466    1.55338   3.1947   L
C-CA--0.234100       0    -10.70722  -0.59057   4.50748  L
C-CA--0.234100       0    -9.74883   0.37743   2.48039  L
C-C-0.322600         0    -10.38852  -0.69121   3.13834  L
O-OH--0.557900       0    -10.71298  -1.82026   2.46487  L
H-H-0.271900         0    -9.01      4.51912   7.23934  L
H-H1-0.087600        0    -10.74716   4.46545   5.07081  L
H-HC-0.029500        0    -8.73507   2.5552    6.17082  L
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H-HC-0.029500        0    -8.72173   3.51094   4.72921  L
H-HA-0.169900        0    -10.57069   0.62919   6.28435  L
H-HA-0.169900        0    -8.95884   2.37547   2.68912  L
H-HA-0.165600        0    -11.20143  -1.40985   5.00075  L
H-HA-0.165600        0    -9.50782   0.28525   1.43     L
H-HO-0.399200        0    -11.61934  -2.0555    2.73142  L
N-N--0.516300        0    -12.00478   2.67775   7.44498  L
C-CT-0.038100        -1   -13.23303   2.11295   7.98099  L
C-C-0.536600         0    -14.4372   3.07207   8.13296  L
O-O--0.581900        0    -15.57235   2.57736   8.17708  L
C-CT--0.030300       0    -12.90853   1.55094   9.38901  L
C-C-0.799400         0    -12.20789   0.18707   9.38897  L
O-O2--0.801400       0    -12.71951  -0.73104   8.70872  L
O-O2--0.801400       0    -11.21536  -0.01928   10.11633  L
H-H-0.293600         0    -11.1766   2.73098   8.03062  L
H-H1-0.088000        0    -13.55163   1.29498   7.3346   L
H-HC--0.012200       0    -13.83911   1.42588   9.94461  L
H-HC--0.012200       0    -12.31172   2.27839   9.93993  L
N-N--0.415700        0    -14.19885   4.3825    8.31483  L
C-CT--0.149000       -1   -15.14982   5.42675   8.7253   L
H-H-0.271900         0    -13.24431   4.68241   8.13221  L
H-H1-0.097600        0    -16.05327   5.35719   8.1174   L
H-H1-0.097600        0    -14.69544   6.40843   8.58026  L
H-H1-0.097600        0    -15.41098   5.29676   9.77587  L
C-CT--0.366200       -1   -19.78818  -1.18541  -1.35732  L
C-C-0.597200         0    -18.79173  -0.82465  -0.24421  L
O-O--0.567900        0    -18.40445   0.33456  -0.17204  L
H-HC-0.112300        0    -20.64512  -1.69945  -0.92909  L
H-HC-0.112300        0    -19.28685  -1.81996  -2.08671  L
H-HC-0.112300        0    -20.11408  -0.26893  -1.84755  L
N-N--0.415700        0    -18.36467  -1.76354   0.62947  L
C-CT--0.058100       -1   -17.24076  -1.53699   1.58781  L
C-C-0.597300         0    -16.39453  -2.7665    1.93164  L
O-O--0.567900        0    -16.82207  -3.58613   2.74936  L
C-CT--0.007400       0    -17.68189  -0.75593   2.8368   L
C-CC-0.186800        0    -16.49853  -0.02033   3.4226   L
N-NB--0.543200       0    -15.45744  -0.62843   4.11532  L
C-CW--0.220700       0    -16.17159   1.28868   3.20945  L
C-CR-0.163500        0    -14.49989   0.3044    4.26245  L
N-NA--0.279500       0    -14.92249   1.47956   3.77252  L
H-H-0.271900         0    -18.71967  -2.70078   0.52691  L
H-H1-0.136000        0    -16.58394  -0.8349    1.07972  L
H-HC-0.036700        0    -18.10751  -1.43176   3.5789   L
H-HC-0.036700        0    -18.43964  -0.02096   2.56352  L
H-H4-0.186200        0    -16.74525   2.00318   2.63301  L
H-H-0.333900         0    -14.35362   2.32466   3.79698  L
H-H5-0.143500        0    -13.53079   0.14388   4.72148  L
N-N--0.254800        0    -15.18891  -2.89611   1.34708  L
C-CT--0.026600       -1   -14.23461  -3.90895   1.76487  L
C-C-0.589600         0    -13.54776  -3.57186   3.07859  L
O-O--0.574800        0    -13.15638  -2.42861   3.31402  L
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C-CT--0.007000       0    -13.18492  -3.9563    0.66325  L
C-CT-0.018900        0    -13.21243  -2.56753   0.02744  L
C-CT-0.019200        0    -14.65664  -2.11986   0.22582  L
H-H1-0.064100        0    -14.72425  -4.88024   1.84601  L
H-HC-0.025300        0    -13.50795  -4.69757  -0.05151  L
H-HC-0.025300        0    -12.19352  -4.21076   1.04135  L
H-HC-0.021300        0    -12.94005  -2.59417  -1.02803  L
H-HC-0.021300        0    -12.54942  -1.89451   0.56895  L
H-H1-0.039100        0    -14.66442  -1.049     0.43082  L
H-H1-0.039100        0    -15.23326  -2.33828  -0.67451  L
N-N--0.347900        0    -13.27861  -4.58608   3.90254  L
C-CT--0.263700      -1    -12.51768  -4.39961   5.14475  L
C-C-0.734100         0    -11.00712  -4.74097   4.97567  L
O-O--0.589400        0    -10.68001  -5.59854   4.16115  L
C-CT--0.000700       0    -13.24269  -5.04535   6.3383   L
C-CT-0.039000        0    -14.56252  -4.29854   6.65957  L
C-CT-0.048600        0    -14.35208  -2.91207   7.30767  L
N-N2--0.529500       0    -15.26635  -1.87153   6.78076  L
C-CA-0.807600        0    -15.68013  -0.77039   7.3932   L
N-N2--0.862700       0    -15.39847  -0.49584   8.62643  L
N-N2--0.862700       0    -16.35268   0.14545   6.76498  L
H-H-0.274700         0    -13.54246  -5.51527   3.60017  L
H-H1-0.156000        0    -12.4951   -3.33328   5.36031  L
H-HC-0.032700        0    -12.59656  -5.0244    7.21787  L
H-HC-0.032700        0    -13.46478  -6.08633   6.10007  L
H-HC-0.028500        0    -15.1477   -4.90785   7.34896  L
H-HC-0.028500        0    -15.14926  -4.19284   5.74585  L
H-H1-0.068700        0    -13.33081  -2.58065   7.12571  L
H-H1-0.068700        0    -14.47156  -3.0124    8.38796  L
H-H-0.345600         0    -15.45516  -1.88562   5.78351  L
H-H-0.447800         0    -15.62827   0.42858   8.94628  L
H-H-0.447800         0    -14.50801  -0.91044   8.9034   L
H-H-0.447800         0    -16.43039   1.0617    7.1902   L
H-H-0.447800         0    -16.38651   0.05334   5.75651  L
N-N--0.415700        0    -10.08333  -4.02344   5.64696  L
C-CT--0.003100      -1    -8.59683   -4.12929   5.53421  L
C-C-0.597300         0    -8.00253   -4.96181   6.67727  L
O-O--0.567900        0    -8.463     -4.88065   7.81784  L
C-CT--0.003600       0    -7.96471   -2.73096   5.49313  L
C-CT--0.064500       0    -6.42966   -2.80615   5.40876  L
C-C-0.695100         0    -5.83817   -1.47735   4.99214  L
O-O--0.608600        0    -6.08406   -1.03225   3.88422  L
N-N--0.940700        0    -5.04063   -0.83149   5.80946  L
H-H-0.271900         0    -10.42968  -3.33547   6.30582  L
H-H1-0.085000        0    -8.36921   -4.64115   4.60533  L
H-HC-0.017100        0    -8.2504    -2.16607   6.37886  L
H-HC-0.017100        0    -8.35046   -2.1973    4.6265   L
H-HC-0.035200        0    -6.13662   -3.54306   4.66181  L
H-HC-0.035200        0    -6.02326   -3.10659   6.37187  L
H-H-0.425100         0    -4.7734     0.12098   5.59068  L
H-H-0.425100         0    -4.71596   -1.31009   6.66043  L
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N-N--0.415700        0    -6.94502  -5.71628   6.37254  L
C-CT--0.001400       -1   -6.19929  -6.53416   7.32412  L
C-C-0.597300         0    -4.6954   -6.47533   7.03499  L
O-O--0.567900        0    -4.25321  -6.65204   5.89391  L
C-CT--0.015200       0    -6.68064  -7.99721   7.26999  L
C-CA--0.001100       0    -8.17763  -8.18624   7.10418  L
C-CA--0.190600       0    -9.02492  -8.3473    8.21978  L
C-CA--0.190600       0    -8.72298  -8.14939   5.8079   L
C-CA--0.234100       0    -10.41727  -8.48597   8.03393  L
C-CA--0.234100       0    -10.10849  -8.26225   5.62788  L
C-C-0.322600         0    -10.95958  -8.4471    6.73146  L
O-OH--0.557900       0    -12.29264  -8.59239   6.5177   L
H-H-0.271900         0    -6.6558   -5.75803   5.39975  L
H-H1-0.087600        0    -6.37405  -6.15007   8.33032  L
H-HC-0.029500        0    -6.35054  -8.50652   8.17603  L
H-HC-0.029500        0    -6.19395  -8.49393   6.42886  L
H-HA-0.169900        0    -8.60822  -8.34886   9.21646  L
H-HA-0.169900        0    -8.08123  -7.98958   4.95089  L
H-HA-0.165600        0    -11.08267  -8.60986   8.87353  L
H-HA-0.165600        0    -10.52886  -8.17301   4.64425  L
H-HO-0.399200        0    -12.43021  -8.69971   5.56419  L
N-N--0.516300        0    -3.89593  -6.2428    8.07344  L
C-CT-0.039700        -1   -2.44492  -6.16548   7.94877  L
C-C-0.536600         0    -1.75769  -7.53952   8.02799  L
O-O--0.581900        0    -1.99131  -8.32707   8.94501  L
C-CT-0.056000        0    -1.8311   -5.18242   8.95305  L
C-CT-0.013600        0    -2.09547  -3.72701   8.54051  L
C-C-0.805400         0    -3.57734  -3.32362   8.63159  L
O-O2--0.818800       0    -4.27174  -3.79928   9.56337  L
O-O2--0.818800       0    -4.03002  -2.53535   7.77304  L
H-H-0.293600         0    -4.3091   -5.93573   8.94621  L
H-H1-0.110500        0    -2.23448  -5.76668   6.96302  L
H-HC--0.017300       0    -0.74909  -5.32695   8.95957  L
H-HC--0.017300       0    -2.2029   -5.37774   9.95991  L
H-HC--0.042500       0    -1.73584  -3.58439   7.5193   L
H-HC--0.042500       0    -1.49274  -3.08397   9.18153  L
N-N--0.415700        0    -0.86066  -7.81908   7.07621  L
C-CT--0.002400       -1   -0.10251  -9.07339   6.97625  L
C-C-0.597300         0     1.39995  -8.83952   7.15471  L
O-O--0.567900        0     1.91713  -7.71834   7.17965  L
C-CT--0.034300       0    -0.44515  -9.76146   5.63544  L
C-CA-0.011800        0     0.11668  -9.07895   4.39576  L
C-CA--0.125600       0    -0.60604  -8.06327   3.74467  L
C-CA--0.125600       0     1.38894  -9.43326   3.9117   L
C-CA--0.170400       0    -0.02817  -7.36006   2.6707   L
C-CA--0.170400       0     1.9704   -8.72973   2.84131  L
C-CA--0.107200       0     1.26152  -7.68694   2.22318  L
H-H-0.271900         0    -0.71972  -7.1131    6.35832  L
H-H1-0.097800        0    -0.42649  -9.7369    7.77883  L
H-HC-0.029500        0    -1.53088  -9.82511   5.54153  L
H-HC-0.029500        0    -0.07238  -10.78561   5.66444  L
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H-HA-0.133000        0    -1.5876   -7.78254   4.10283  L
H-HA-0.133000        0     1.92584  -10.24063   4.37854  L
H-HA-0.143000        0    -0.55826  -6.53788   2.211    L
H-HA-0.143000        0     2.96133  -8.9822    2.49744  L
H-HA-0.129700        0     1.70294  -7.12303   1.4143   L
N-N--0.415700        0     2.13106  -9.94191   7.30249  L
C-CT--0.024900       -1    3.57461  -9.89397   7.49388  L
C-C-0.597300         0     4.3269   -9.40804   6.23806  L
O-O--0.567900        0     4.20443  -9.97865   5.15652  L
C-CT-0.211700        0     4.11813  -11.26792   7.92578  L
O-OH--0.654600       0     3.86825  -12.29922   6.97663  L
H-H-0.271900         0     1.64982  -10.82316   7.23927  L
H-H1-0.084300        0     3.78131  -9.19272   8.30334  L
H-H1-0.035200        0     3.66689  -11.54471   8.88018  L
H-H1-0.035200        0     5.19583  -11.18368   8.07531  L
H-HO-0.427500        0     3.09782  -12.79641   7.27983  L
N-N--0.347900        0     5.17973  -8.38974   6.37893  L
C-CT--0.263700       -1    6.07737  -7.87252   5.32155  L
C-C-0.734100         0     7.16078  -8.87458   4.88702  L
O-O--0.589400        0     7.21178  -10.01437   5.35523  L
C-CT--0.000700       0     6.6408   -6.5281    5.83475  L
C-CT-0.039000        0     7.75962  -6.65101   6.8857   L
C-CT-0.048600        0     8.10337  -5.31263   7.55574  L
N-N2--0.529500       0     8.42341  -4.24008   6.58904  L
C-CA-0.807600        0     7.66314  -3.21081   6.25679  L
N-N2--0.862700       0     6.44666  -3.10655   6.69353  L
N-N2--0.862700       0     8.09424  -2.24969   5.49853  L
H-H-0.274700         0     5.16673  -7.93319   7.27751  L
H-H1-0.156000        0     5.4642   -7.66731   4.44112  L
H-HC-0.032700        0     5.81756  -5.94552   6.25283  L
H-HC-0.032700        0     7.03068  -5.95934   4.99957  L
H-HC-0.028500        0     8.65899  -7.03885   6.41079  L
H-HC-0.028500        0     7.45474  -7.35193   7.66334  L
H-H1-0.068700        0     8.96973  -5.46786   8.2012   L
H-H1-0.068700        0     7.27379  -5.01476   8.19852  L
H-H-0.345600         0     9.35916  -4.23743   6.19112  L
H-H-0.447800         0     5.90136  -2.2689    6.44863  L
H-H-0.447800         0     6.03769  -3.77389   7.30403  L
H-H-0.447800         0     7.42016  -1.49403   5.35512  L
H-H-0.447800         0     8.99703  -2.24526   5.05085  L
N-N--0.415700        0     8.04539  -8.42905   4.00418  L
C-CT--0.051800       -1    9.37453  -8.97246   3.73158  L
C-C-0.597300         0     10.31783  -7.78145   3.88714  L
O-O--0.567900        0     10.41751  -6.9252    3.01419  L
C-CT--0.110200       0     9.3718   -9.61535   2.32797  L
C-CT-0.353100        0     10.67457  -10.31696   1.88925  L
C-CT--0.412100       0     10.35115  -11.34155   0.79862  L
C-CT--0.412100       0     11.71694  -9.36943   1.29716  L
H-H-0.271900         0     7.86236  -7.51405   3.59959  L
H-H1-0.092200        0     9.63434  -9.73435   4.46891  L
H-HC-0.045700        0     9.08938  -8.87512   1.57803  L
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H-HC-0.045700        0     8.59131  -10.36923   2.34231  L
H-HC--0.036100       0     11.10541  -10.84349   2.74105  L
H-HC-0.100000        0     11.2632  -11.85459   0.49203  L
H-HC-0.100000        0     9.92085  -10.83803  -0.06945  L
H-HC-0.100000        0     9.6497   -12.08471   1.17434  L
H-HC-0.100000        0     12.57732  -9.93844   0.9462   L
H-HC-0.100000        0     12.06147  -8.66289   2.04368  L
H-HC-0.100000        0     11.28777  -8.81929   0.46056  L
N-N--0.415700        0     10.96687  -7.68334   5.0411   L
C-CT-0.014300        -1    12.2554  -7.0175    5.07656  L
C-C-0.597300         0     13.28733  -8.08643   4.62745  L
O-O--0.567900        0     13.27533  -9.17361   5.20552  L
C-CT--0.204100       0     12.60378  -6.53904   6.49745  L
C-C-0.713000         0     11.84362  -5.31326   6.9597   L
O-O--0.593100        0     11.15676  -4.62899   6.2187   L
N-N--0.919100        0     11.94202  -4.98747   8.22638  L
H-H-0.271900         0     10.85482  -8.44383   5.6937   L
H-H1-0.104800        0     12.29007  -6.17481   4.384    L
H-HC-0.079700        0     13.66468  -6.28472   6.51944  L
H-HC-0.079700        0     12.442   -7.35278   7.20458  L
H-H-0.419600         0     11.48652  -4.13837   8.50408  L
H-H-0.419600         0     12.55071  -5.50838   8.83618  L
N-N--0.415700        0     14.12373  -7.84338   3.6071   L
C-CT--0.051800       -1    15.22917  -8.75434   3.25005  L
C-C-0.597300         0     16.44112  -8.5228    4.19092  L
O-O--0.567900        0     16.7101  -7.38175   4.56249  L
C-CT--0.110200       0     15.59734  -8.61994   1.73838  L
C-CT-0.353100        0     16.6221  -9.64828   1.17352  L
C-CT--0.412100       0     16.13551  -11.08888   1.36969  L
C-CT--0.412100       -1    16.90716  -9.49697  -0.34105  L
H-H-0.271900         0     14.09383  -6.94895   3.14026  L
H-H1-0.092200        0     14.88012  -9.77234   3.41899  L
H-HC-0.045700        0     15.99507  -7.62029   1.56731  L
H-HC-0.045700        0     14.68179  -8.70641   1.15418  L
H-HC--0.036100       0     17.56411  -9.52917   1.70407  L
H-HC-0.100000        0     15.1605  -11.22214   0.90143  L
H-HC-0.100000        0     16.06922  -11.32825   2.42844  L
H-HC-0.100000        0     16.8483  -11.7795   0.91823  L
H-HC-0.100000        0     16.01221  -9.7234   -0.91673  L
H-HC-0.100000        0     17.7102  -10.17369  -0.63302  L
H-HC-0.100000        0     17.2281  -8.47406  -0.54179  L
N-N--0.516300        0     17.16651  -9.57846   4.59179  L
C-CT-0.039700        -1    18.41967  -9.44882   5.37424  L
C-C-0.536600         0     19.5024  -8.64399   4.59767  L
O-O--0.581900        0     19.43692  -8.52244   3.37124  L
C-CT-0.056000        0     18.95359  -10.82026   5.83098  L
C-CT-0.013600        0     18.65353  -11.08568   7.31626  L
C-C-0.805400         0     19.21164  -10.00192   8.26066  L
O-O2--0.818800       0     18.68829  -9.90571   9.39022  L
O-O2--0.818800       0     20.10478  -9.23528   7.82359  L
H-H-0.293600         0     16.91158  -10.49402   4.26628  L
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H-H1-0.110500        0     18.18536  -8.845     6.2518   L
H-HC--0.017300       0     20.03383  -10.86471   5.68428  L
H-HC--0.017300       0     18.51035  -11.6132   5.22577  L
H-HC--0.042500       0     19.07996  -12.05422   7.58676  L
H-HC--0.042500       0     17.56944  -11.15228   7.43782  L
N-N--0.415700        0     20.46684  -8.02245   5.29452  L
C-CT--0.025200       -1    21.47464  -7.09007   4.72744  L
C-C-0.597300         0     20.8605  -5.82484   4.06314  L
O-O--0.567900        0     21.60955  -5.05876   3.46085  L
H-H-0.271900         0     20.48734  -8.23881   6.2956   L
H-H1-0.069800        0     22.06002  -7.61538   3.97298  L
H-H1-0.069800        0     22.14737  -6.76619   5.52068  L
N-N--0.415700        0     19.5349  -5.57337   4.13986  L
C-CT--0.038900       0     18.80366  -4.67254   3.20824  L
C-C-0.597300         0     17.83516  -3.66984   3.87942  L
O-O--0.567900        0     17.01244  -4.01536   4.72471  L
C-CT-0.365400        0     18.0124  -5.49788   2.1709   L
O-OH--0.676100       0     18.78734  -6.52473   1.59359  L
C-CT--0.243800       0     17.55109  -4.6549    0.98034  L
H-H-0.271900         0     18.97593  -6.23057   4.66895  L
H-H1-0.100700        0     19.54152  -4.09614   2.65164  L
H-H1-0.004300        0     17.13708  -5.93473   2.64507  L
H-HC-0.064200        0     16.89214  -3.85418   1.30626  L
H-HC-0.064200        0     17.0058  -5.29071   0.28259  L
H-HC-0.064200        0     18.41628  -4.23128   0.46972  L
H-HO-0.410200        0     19.0135  -7.17969   2.28113  L
N-N--0.415700        0     17.87494  -2.39946   3.45085  L
C-CT--0.087500       -1    16.96512  -1.2941    3.85085  L
C-C-0.597300         0     15.60277  -1.43255   3.13486  L
O-O--0.567900        0     15.55709  -1.44322   1.90808  L
C-CT-0.298500        0     17.56085   0.07583   3.44012  L
C-CT--0.319200       -1    16.68983   1.27929   3.90165  L
C-CT--0.319200       -1    19.00489   0.17692   3.9627   L
H-H-0.271900         0     18.55698  -2.19782   2.73522  L
H-H1-0.096900        0     16.82012  -1.31778   4.93033  L
H-HC--0.029700       0     17.6222   0.12097   2.35239  L
H-HC-0.079100        0     16.57146   1.2615    4.98432  L
H-HC-0.079100        0     15.71435   1.25383   3.41668  L
H-HC-0.079100        0     17.18553   2.20773   3.61539  L
H-HC-0.079100        0     19.02809   0.00773   5.03949  L
H-HC-0.079100        0     19.39441   1.17393   3.75455  L
H-HC-0.079100        0     19.65657  -0.54104   3.46544  L
N-N--0.415700        0     14.48071  -1.54397   3.86458  L
C-CT--0.023700       -1    13.1784  -1.97569   3.29142  L
C-C-0.597300         0     11.91218  -1.34145   3.94623  L
O-O--0.567900        0     10.81231  -1.90745   3.92476  L
C-CT-0.034200        0     13.0723  -3.50989   3.5048   L
C-CT-0.001800        0     14.16937  -4.41671   2.92269  L
S-S--0.273700        0     13.7158  -5.31256   1.41424  L
C-CT--0.053600       0     13.82493  -3.96183   0.21615  L
H-H-0.271900         0     14.61746  -1.61912   4.86031  L
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 H-H1-0.088000        0     13.14082  -1.762     2.22244  L
 H-HC-0.024100        0     12.1189  -3.86774   3.11335  L
 H-HC-0.024100        0     13.05955  -3.68335   4.58122  L
 H-H1-0.044000        0     14.41551  -5.15816   3.68203  L
 H-H1-0.044000        0     15.0821  -3.86134   2.73703  L
 H-H1-0.068400        0     14.82299  -3.52437   0.23697  L
 H-H1-0.068400        0     13.09192  -3.19308   0.45576  L
 H-H1-0.068400        0     13.62541  -4.35522  -0.7779   L
 N-N--0.415700        0     12.03977  -0.14862   4.53041  L
 C-CT--0.024900       -1    10.92267   0.76211   4.86052  L
 C-C-0.597300         0     11.01348   1.87913   3.82676  L
 O-O--0.567900        0     12.10499   2.41205   3.62787  L
 C-CT-0.211700        0     11.05668   1.23887   6.30278  L
 O-OH--0.654600       0     10.14305   2.26357   6.65095  L
 H-H-0.271900         0     12.9477   0.28204   4.42492  L
 H-H1-0.084300        0     9.96394   0.25438   4.74792  L
 H-H1-0.035200        0     12.06909   1.60464   6.43325  L
 H-H1-0.035200        0     10.90636   0.38723   6.96791  L
 H-HO-0.427500        0     9.25251   2.01117   6.30028  L
 N-N--0.347900        0     9.93411   2.15976   3.08593  L
 C-CT--0.240000       -1    9.97867   3.0625    1.92055  L
 C-C-0.734100         0     10.52844   4.44813   2.34137  L
 O-O--0.589400        0     11.56511   4.82744   1.80173  L
 C-CT--0.009400       0     8.60752   3.08676   1.23309  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.60442   3.85152  -0.09884  H
 C-CT--0.047900       0     7.50866   3.33793  -1.03103  H
 C-CT--0.014300       0     7.3702    4.16644  -2.29201  H
 N-N3--0.385400       0     6.36965   3.57127  -3.19637  H
 H-H-0.274700         0     9.06432   1.69128   3.3147   L
 H-H1-0.142600        0     10.69857   2.6579    1.20721  L
 H-HC-0.036200        0     7.87254   3.52753   1.89986  L
 H-HC-0.036200        0     8.30992   2.05356   1.04168  L
 H-HC-0.010300        0     9.58134   3.73388  -0.57958  H
 H-HC-0.010300        0     8.46663   4.9165    0.12012  H
 H-HC-0.062100        0     6.52826   3.32493  -0.54691  H
 H-HC-0.062100        0     7.7187    2.30362  -1.33128  H
 H-HP-0.113500        0     8.33674   4.3052   -2.79541  H
 H-HP-0.113500        0     7.00914   5.17297  -2.04556  H
 H-H-0.340000         0     6.80201   3.0066   -3.93176  H
 H-H-0.340000         0     6.01082   4.33783  -3.80129  H
 H-H-0.340000         0     3.61471   2.78377  -0.87753  H
 N-N--0.347900        0     9.9953    5.11297   3.39543  L
 C-CT--0.263700       -1    10.62414   6.26496   4.13441  L
 C-C-0.734100         0     11.76283   5.8433    5.03941  L
 O-O--0.589400        0     11.74194   6.10667   6.24488  L
 C-CT--0.000700       0     9.54073   7.15914   4.77458  L
 C-CT-0.039000        0     8.71617   7.83725   3.66007  L
 C-CT-0.048600        0     7.71613   8.89907   4.13306  L
 N-N2--0.529500       0     6.66207   8.36801   5.01763  L
 C-CA-0.807600        0     5.41748   8.80197   5.12069  L
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N-N2--0.862700       0     4.90446   9.68255   4.31233  L
N-N2--0.862700       0     4.68281   8.34761   6.0848   L
H-H-0.274700         0     9.10099   4.76299   3.72583  L
H-H1-0.156000        0     11.11916   6.8921    3.38644  L
H-HC-0.032700        0     10.02018   7.93768   5.37034  L
H-HC-0.032700        0     8.89488   6.56384   5.42083  L
H-HC-0.028500        0     8.18218   7.08169   3.08823  L
H-HC-0.028500        0     9.4049    8.33343   2.97492  L
H-H1-0.068700        0     7.26083   9.33124   3.24047  L
H-H1-0.068700        0     8.25549   9.69135   4.65465  L
H-H-0.345600         0     6.87486   7.61155   5.65332  L
H-H-0.447800         0     3.92138   9.95646   4.38217  L
H-H-0.447800         0     5.41615   9.96561   3.49758  L
H-H-0.447800         0     3.76037   8.75651   6.24571  L
H-H-0.447800         0     5.02323   7.62004   6.68625  L
N-N--0.347900        0     12.72012   5.17148   4.38183  L
C-CT--0.240000       -1    14.11386   4.81019   4.70412  L
C-C-0.734100         0     14.97048   4.52976   3.43766  L
O-O--0.589400        0     16.182    4.69075   3.50746  L
C-CT--0.009400       0     14.2918   3.65542   5.73154  L
C-CT-0.018700        0     13.45186   3.95877   6.96828  L
C-CT--0.047900       0     13.5107   3.13922   8.25933  L
C-CT--0.014300       0     12.49616   3.72184   9.27917  L
N-N3--0.385400       0     11.18198   4.1232    8.68325  L
H-H-0.274700         0     12.46411   5.09525   3.40418  L
H-H1-0.142600        0     14.57381   5.69673   5.14485  L
H-HC-0.036200        0     15.34301   3.59332   6.01791  L
H-HC-0.036200        0     13.99168   2.70198   5.29912  L
H-HC-0.010300        0     12.43889   3.84411   6.6014   L
H-HC-0.010300        0     13.65836   4.9903    7.25684  L
H-HC-0.062100        0     14.51641   3.19386   8.67969  L
H-HC-0.062100        0     13.28224   2.09406   8.06178  L
H-HP-0.113500        0     12.95385   4.60407   9.73726  L
H-HP-0.113500        0     12.34044   2.98461   10.07198  L
H-H-0.340000         0     11.31805   4.87599   8.00758  L
H-H-0.340000         0     10.52461   4.44307   9.38082  L
H-H-0.340000         0     10.75924   3.36061   8.15376  L
N-N--0.415700        0     14.38007   4.09588   2.31153  L
C-CT--0.051800       -1    15.04441   3.67907   1.04685  L
C-C-0.597300         0     15.26934   4.77891   0.04507  L
O-O--0.567900        0     16.2482   4.75352  -0.69863  L
C-CT--0.110200       0     14.19637   2.52605   0.46681  L
C-CT-0.353100        0     14.74447   1.85394  -0.80756  L
C-CT--0.412100       0     16.12901   1.2387   -0.59896  L
C-CT--0.412100       0     13.79074   0.73439  -1.23356  L
H-H-0.271900         0     13.37874   3.96142   2.35983  L
H-H1-0.092200        0     16.02971   3.28564   1.30168  L
H-HC-0.045700        0     13.20006   2.91221   0.2449   L
H-HC-0.045700        0     14.09015   1.75897   1.23605  L
H-HC--0.036100       0     14.79445   2.58446  -1.61428  L
H-HC-0.100000        0     16.10793   0.53374   0.23125  L
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H-HC-0.100000        0     16.85858   2.02192  -0.39544  L
H-HC-0.100000        0     16.43924   0.71705  -1.50398  L
H-HC-0.100000        0     14.14609   0.28776  -2.16204  L
H-HC-0.100000        0     12.79387   1.14117  -1.40126  L
H-HC-0.100000        0     13.74503  -0.03466  -0.46128  L
N-N--0.415700        0     14.36217   5.73998   0.02658  L
C-CT-0.014300       -1     14.56638   6.94874  -0.72652  L
C-C-0.597300         0     15.64189   7.87805  -0.09009  L
O-O--0.567900        0     15.34148   8.96499   0.39693  L
C-CT--0.204100       0     13.20102   7.62829  -1.0065   L
C-C-0.713000         0     12.21838   7.73339   0.15767  L
O-O--0.593100        0     12.53438   7.59194   1.33073  L
N-N--0.919100        0     10.95506   7.93674  -0.14346  L
H-H-0.271900         0     13.6014   5.71807   0.69511  L
H-H1-0.104800        0     14.9697   6.67709  -1.70379  L
H-HC-0.079700        0     12.7048   7.06073  -1.79318  L
H-HC-0.079700        0     13.37576   8.63328  -1.38926  L
H-H-0.419600         0     10.32185   7.98243   0.62856  L
H-H-0.419600         0     10.62318   8.0309   -1.10224  L
N-N--0.415700        0     16.916    7.45136  -0.14346  L
C-CT--0.149000      -1     18.10837   8.14328   0.36256  L
H-H-0.271900         0     17.0316   6.52014  -0.53036  L
H-H1-0.097600        0     18.09346   8.14393   1.4538   L
H-H1-0.097600        0     18.10987   9.17683   0.01098  L
H-H1-0.097600        0     19.01046   7.63985   0.01286  L
C-CT--0.055800       0     0.79733   15.01854   4.42788  L
C-CT-0.000000        0     1.13614   14.12257   3.2385   L
O-OS--0.354800       0     2.52401   14.21243   2.95378  L
C-CT--0.202200       0     0.85732   12.6506   3.55131  L
O-OS--0.524600       0     0.32203   12.07207   2.36105  L
C-CT--0.067000       0     2.24655   12.12457   3.89033  L
O-OH--0.613900       0     2.32836   10.72773   3.74409  L
C-CT--0.006600       0     2.99545   12.88557   2.81163  L
N-N*--0.048400       0     4.46694   12.77895   2.94067  L
C-C-0.753800         0     5.15135   11.93908   2.05766  L
O-O--0.625200        0     4.57282   11.34804   1.14956  L
N-NC--0.758400       0     6.48621   11.73639   2.20967  L
C-CA-0.818500        0     7.11545   12.39393   3.15494  L
N-N2--0.953000       0     8.40137   12.19462   3.19049  L
C-CM--0.521500       0     6.48023   13.25385   4.08716  L
C-CM--0.005300       0     5.1395    13.41822   3.95222  L
H-H1-0.067900        0    -0.2789    14.99504   4.59707  L
H-H1-0.067900        0     1.30935   14.65102   5.31713  L
H-H1-0.117400        0     0.5359    14.42634   2.37649  L
H-H1-0.061500        0     0.15498   12.56368   4.37894  L
H-H1-0.097200        0     2.54824   12.44739   4.88926  L
H-HO-0.418600        0     1.60345   10.49358   3.13606  L
H-H2-0.202900        0     2.66352   12.48342   1.84989  L
H-H-0.423400         0     8.738     11.67528   2.40112  L
H-H-0.423400         0     8.97199   12.74544   3.79966  L
H-HA-0.192800        0     7.00831   13.7695   4.87118  L
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 H-H4-0.195800        0     4.57926   14.05586   4.62739  L
 P-P-1.166200         0    -0.621     10.76511   2.33791  L
 O-O2--0.776000       0    -1.62765   10.89836   1.26604  L
 O-O2--0.776000       0    -1.03598   10.42826   3.71686  L
 O-OS--0.498900       0     0.41387   9.62193   1.90106  L
 C-CT-0.055800        0     1.178     9.7194    0.70967  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     1.96614   8.41804   0.47408  H
 O-OS--0.354800       0     2.72017   8.14307   1.64759  H
 C-CT-0.202200        0     1.09511   7.19162   0.13834  H
 O-OH--0.654100       0     1.38741   6.62495  -1.12478  H
 C-CT-0.067000        0     1.47202   6.14438   1.229    H
 O-OH--0.613900       0     1.99613   4.91946   0.73681  H
 C-CT-0.039400        0     2.64055   6.78341   2.00338  H
 N-N*--0.025100       0     2.4886    6.70654   3.43128  H
 C-CK-0.200600        0     1.60162   7.42581   4.21769  H
 N-NB--0.607300       0     1.60476   7.05384   5.46916  H
 C-CB-0.051500        0     2.51547   6.02148   5.51757  H
 C-CA-0.700900        0     2.91543   5.15543   6.55315  H
 N-N2--0.901900       0     2.44814   5.27575   7.82653  H
 N-NC--0.761500       0     3.87484   4.25163   6.29707  H
 C-CQ-0.587500        0     4.25447   4.08241   5.03007  H
 N-NC--0.699700       0     3.95511   4.82507   3.97228  H
 C-CB-0.305300        0     3.07781   5.78782   4.2649   H
 H-H1-0.067900        0     1.8767    10.55164   0.79943  L
 H-H1-0.067900        0     0.51925   9.90444  -0.14121  L
 H-H1-0.117400        0     2.63911   8.56238  -0.37798  H
 H-H1-0.061500        0     0.02952   7.43896   0.20631  H
 H-HO-0.437600        0     1.03031   7.1907   -1.84601  H
 H-H1-0.097200        0     0.61598   5.98351   1.89229  H
 H-HO-0.418600        0     5.15527   4.15499   0.9673   H
 H-H2-0.200700        0     3.55562   6.25927   1.72511  H
 H-H5-0.155300        0     1.00327   8.22471   3.79262  H
 H-H-0.411500         0     2.39039   4.38479   8.33228  H
 H-H-0.411500         0     1.569     5.78187   7.89575  H
 H-H5-0.047300        0     4.94986   3.27194   4.84157  H
 N-N3-0.149300        0    -0.94365   4.98455  -0.34345  H
 C-CT-0.053600        0    -0.28011   3.94328   0.48176  H
 C-CT-0.065100        0    -0.87439   2.55453   0.21352  H
 C-CT--0.090300       0    -0.60359   1.51905   1.31565  H
 C-C-0.735400         0    -1.54646   0.32297   1.1995   H
 O-O--0.613300        0    -1.18071  -0.80923   0.95643  H
 N-N--1.003100        0    -2.89382   0.64438   1.2943   H
 C-C-0.612300         0     1.20724   3.97207   0.14624  H
 O-O--0.571300        0     1.72246   3.17382  -0.58646  H
 O-OS--0.421200       0     2.68732   1.41847   1.24215  H
 P-P-1.166200         0     4.00905   1.23267   0.61822  H
 O-O2--0.776000       0     5.28747   1.28348   1.54353  H
 O-O2--0.776000       0     4.38296   2.28444  -0.53358  H
 O-OS--0.498900       0     4.22597  -0.18997  -0.07701  H
 C-CT-0.055800        0     3.32277  -0.51973  -1.15027  H
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 C-CT-0.106500        0     2.65299  -1.88623  -0.91663  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.57018  -2.89628  -0.48277  L
 C-CT-0.039400        0     3.39942  -3.09662   0.92354  L
 N-N*--0.025100       0     4.72025  -3.07067   1.60419  L
 C-CB-0.305300        0     5.48697  -4.18049   1.85305  L
 N-NC--0.699700       0     5.14583  -5.47905   1.62102  L
 C-CQ-0.587500        0     6.10911  -6.31187   1.97432  L
 N-NC--0.761500       0     7.30123  -6.02806   2.48295  L
 C-CA-0.700900        0     7.60827  -4.74252   2.6518   L
 N-N2--0.901900       0     8.83738  -4.54638   3.09227  L
 C-CB-0.051500        0     6.67197  -3.72514   2.36743  L
 N-NB--0.607300       0     6.66738  -2.33513   2.49978  L
 C-CK-0.200600        0     5.46872  -2.01321   2.07566  L
 C-CT-0.067000        0     2.37222  -2.0803    1.43075  L
 O-OH--0.613900       0     1.57044  -2.58171   2.48483  L
 C-CT-0.202200        0     1.57327  -1.82043   0.1542   L
 O-OH--0.654100       0     0.60266  -2.83833  -0.07841  L
 H-H-0.199600         0    -1.89699   3.99105  -1.65376  H
 H-H-0.199600         0    -0.27959   5.5226   -0.89481  H
 H-H-0.199600         0    -1.4707    5.63243   0.23562  H
 H-HP-0.101500        0    -0.40075   4.18631   1.54702  H
 H-HC-0.005000        0    -0.49153   2.18836  -0.74203  H
 H-HC-0.005000        0    -1.95067   2.67913   0.08071  H
 H-HC-0.033100        0    -0.77998   1.98064   2.29869  H
 H-HC-0.033100        0     0.42884   1.16429   1.29107  H
 H-H-0.442900         0    -3.48377  -0.14098   1.53476  H
 H-H-0.442900         0    -3.08747   1.43803   1.91785  H
 H-H1-0.067900        0     3.89719  -0.56228  -2.0779   H
 H-H1-0.067900        0     2.54014   0.23273  -1.26866  H
 H-H1-0.117400        0     2.178    -2.17288  -1.85528  L
 H-H2-0.200700        0     2.95284  -4.08036   1.07673  L
 H-H5-0.047300        0     5.89202  -7.35975   1.83255  L
 H-H-0.411500         0     9.1865   -3.60497   3.17786  L
 H-H-0.411500         0     9.44554  -5.359     3.10277  L
 H-H5-0.155300        0     5.11383  -0.99563   2.06436  L
 H-H1-0.097200        0     2.85687  -1.15794   1.74223  L
 H-HO-0.418600        0     2.11917  -2.63874   3.29265  L
 H-H1-0.061500        0     1.11029  -0.83436   0.17181  L
 H-HO-0.437600        0    -0.17019  -2.52376   0.42734  L
 O-OW--0.834000       0    -10.34254  -2.08013   11.53741  L
 H-HW-0.417000        0    -10.65024  -1.23615   11.12827  L
 H-HW-0.417000        0    -10.61688  -2.73708   10.87307  L
 O-OW--0.834000       0    -10.29474  -3.84497   9.46732  L
 H-HW-0.417000        0    -10.55042  -3.20499   8.77575  L
 H-HW-0.417000        0    -9.66083  -4.4149    8.99051  L
 O-OW--0.834000       0    -10.74517  -1.9488    7.61165  L
 H-HW-0.417000        0    -11.54433  -1.54145   8.03323  L
 H-HW-0.417000        0    -10.1054  -1.23276   7.69028  L
 O-OW--0.834000       0     5.34389   3.83715   1.87284  H
 H-HW-0.417000        0     4.64251   4.2443    2.44486  H
```

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H-HW-0.417000        0     5.38178   2.25821   1.78069  H
O-OW--0.834000       0     6.9718    4.85999   4.00457  H
H-HW-0.417000        0     6.66833   4.34279   3.2347   H
H-HW-0.417000        0     6.52902   5.69827   3.75512  H
O-OW--0.834000       0     6.4013    2.27887  -5.70868  L
H-HW-0.417000        0     7.29169   2.02048  -6.01218  L
H-HW-0.417000        0     6.25347   3.13134  -6.1391   L
O-OW--0.834000       0     6.35931   5.84054   6.53892  L
H-HW-0.417000        0     5.59193   5.32272   6.83587  L
H-HW-0.417000        0     6.60399   5.39218   5.70981  L
O-OW--0.834000       0     7.78996   1.61444   5.5302   H
H-HW-0.417000        0     7.1301    2.29128   5.31185  H
H-HW-0.417000        0     7.17299   0.86067   5.75429  H
O-OW--0.834000       0     5.67796   6.84943   2.40217  H
H-HW-0.417000        0     5.23292   7.65816   2.09031  H
H-HW-0.417000        0     5.77491   6.38379   1.55081  H
O-OW--0.834000       0     3.70599   16.4898   3.9248   L
H-HW-0.417000        0     3.29967   15.68037   3.57633  L
H-HW-0.417000        0     2.95949   17.07832   4.0388   L
O-OW--0.834000       0    -4.43303   2.14525   5.8272   L
H-HW-0.417000        0    -4.29329   2.10368   6.77806  L
H-HW-0.417000        0    -4.89196   3.02364   5.72725  L
O-OW--0.834000       0     0.2024    1.87424   12.13109  L
H-HW-0.417000        0    -0.18884   1.69033   13.00847  L
H-HW-0.417000        0     0.01476   2.81041   12.03031  L
O-OW--0.834000       0    -2.49857   10.03093   5.88242  L
H-HW-0.417000        0    -2.33009   9.11998   6.20022  L
H-HW-0.417000        0    -2.00719   10.08041   5.0289   L
O-OW--0.834000       0     2.20404   9.42528   6.85446  L
H-HW-0.417000        0     1.72505   8.64207   6.53454  L
H-HW-0.417000        0     1.52675   10.1271   6.74454  L
O-OW--0.834000       0    -5.051     9.10356   5.50986  L
H-HW-0.417000        0    -4.93612   8.21741   5.90758  L
H-HW-0.417000        0    -4.20762   9.54618   5.7134   L
O-OW--0.834000       0    -2.49987   7.54296   7.01186  L
H-HW-0.417000        0    -3.33612   7.07505   6.78287  L
H-HW-0.417000        0    -2.26109   7.16115   7.873    L
O-OW--0.834000       0     0.07587   10.96497   6.28565  L
H-HW-0.417000        0     0.07814   11.02218   5.31342  L
H-HW-0.417000        0    -0.85849   10.77171   6.46364  L
O-O2--0.818800       0     5.31326   7.86852  -0.22247  H
```

## GlnRS in silico Glu34Gln mutant

**Table S2.** Cartesian coordinates and partial charges of all GlnRS Glu34Gln mutant species presently optimized using the ONIOM(QM/MM) approach.

**RC**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.51395 | -11.75904 | -5.43171 | L |
| C-C-0.597200 | 0 | -11.82523 | -10.75217 | -6.32338 | L |
| O-O--0.567900 | 0 | -11.41546 | -11.11683 | -7.41639 | L |
| H-HC-0.112300 | 0 | -11.9237 | -11.89517 | -4.52841 | L |
| H-HC-0.112300 | 0 | -12.58421 | -12.70514 | -5.96631 | L |
| H-HC-0.112300 | 0 | -13.51207 | -11.39907 | -5.19204 | L |
| N-N--0.415700 | 0 | -11.66726 | -9.51935 | -5.83188 | L |
| C-CT--0.058100 | -1 | -10.80859 | -8.49179 | -6.44008 | L |
| C-C-0.597300 | 0 | -9.78421 | -7.96264 | -5.43049 | L |
| O-O--0.567900 | 0 | -10.05846 | -7.8813 | -4.22677 | L |
| C-CT--0.007400 | 0 | -11.61965 | -7.39872 | -7.13114 | L |
| C-CC-0.186800 | 0 | -11.02208 | -6.92325 | -8.42965 | L |
| N-NB--0.543200 | 0 | -11.41793 | -7.33995 | -9.70017 | L |
| C-CW--0.220700 | 0 | -10.15572 | -5.87991 | -8.5522 | L |
| C-CR-0.163500 | 0 | -10.83525 | -6.48847 | -10.55702 | L |
| N-NA--0.279500 | 0 | -10.07472 | -5.60037 | -9.89762 | L |
| H-H-0.271900 | 0 | -12.05799 | -9.30571 | -4.9304 | L |
| H-H1-0.136000 | 0 | -10.23785 | -8.98482 | -7.22912 | L |
| H-HC-0.036700 | 0 | -11.68382 | -6.54571 | -6.46546 | L |
| H-HC-0.036700 | 0 | -12.62864 | -7.75745 | -7.33932 | L |
| H-H4-0.186200 | 0 | -9.73129 | -5.29875 | -7.74919 | L |
| H-H-0.333900 | 0 | -9.72759 | -4.72349 | -10.30543 | L |
| H-H5-0.143500 | 0 | -11.01628 | -6.46758 | -11.62227 | L |
| N-N--0.415700 | 0 | -8.5932 | -7.62754 | -5.92116 | L |
| C-CT--0.038900 | -1 | -7.4385 | -7.10932 | -5.16593 | L |
| C-C-0.597300 | 0 | -6.67245 | -6.03072 | -5.96816 | L |
| O-O--0.567900 | 0 | -7.02039 | -5.7319 | -7.10996 | L |
| C-CT-0.365400 | 0 | -6.44245 | -8.22928 | -4.79962 | L |
| O-OH--0.676100 | 0 | -6.14894 | -9.01311 | -5.91669 | L |
| C-CT--0.243800 | -1 | -6.95041 | -9.16964 | -3.72453 | L |
| H-H-0.271900 | 0 | -8.43914 | -7.83205 | -6.90263 | L |
| H-H1-0.100700 | 0 | -7.77242 | -6.66999 | -4.23353 | L |
| H-H1-0.004300 | 0 | -5.51693 | -7.78874 | -4.42892 | L |
| H-HC-0.064200 | 0 | -7.23226 | -8.60014 | -2.83882 | L |
| H-HC-0.064200 | 0 | -6.16719 | -9.8774 | -3.45743 | L |
| H-HC-0.064200 | 0 | -7.82074 | -9.71492 | -4.09069 | L |
| H-HO-0.410200 | 0 | -5.44104 | -9.64106 | -5.6993 | L |
| N-N--0.347900 | 0 | -5.60016 | -5.44036 | -5.40353 | L |
| C-CT--0.263700 | -1 | -4.61799 | -4.59455 | -6.13043 | L |
| C-C-0.734100 | 0 | -3.21916 | -4.6408 | -5.52657 | L |
| O-O--0.589400 | 0 | -3.09588 | -4.84113 | -4.32361 | L |
| C-CT--0.000700 | 0 | -5.13109 | -3.14634 | -6.26785 | L |
| C-CT-0.039000 | 0 | -4.91864 | -2.20408 | -5.06811 | L |
| C-CT-0.048600 | 0 | -5.7114 | -2.50186 | -3.79238 | L |
| N-N2--0.529500 | 0 | -5.1032 | -3.54406 | -2.95832 | L |
| C-CA-0.807600 | 0 | -5.07672 | -3.60503 | -1.64596 | L |

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 N-N2--0.862700       0    -5.75608  -2.81983  -0.86519  L
 N-N2--0.862700       0    -4.31655  -4.4982   -1.0943   L
 H-H-0.274700         0    -5.36863  -5.73541  -4.46709  L
 H-H1-0.156000        0    -4.54899  -5.01581  -7.12987  L
 H-HC-0.032700        0    -6.19019  -3.15565  -6.52984  L
 H-HC-0.032700        0    -4.60839  -2.69852  -7.11454  L
 H-HC-0.028500        0    -5.23722  -1.22051  -5.39339  L
 H-HC-0.028500        0    -3.85926  -2.12893  -4.83221  L
 H-H1-0.068700        0    -6.72997  -2.77609  -4.06226  L
 H-H1-0.068700        0    -5.7336   -1.57755  -3.21393  L
 H-H-0.345600         0    -4.46254  -4.17357  -3.41694  L
 H-H-0.447800         0    -5.79654  -2.9439    0.13514  L
 H-H-0.447800         0    -6.4914   -2.22017  -1.2645   L
 H-H-0.447800         0    -4.02791  -4.34851  -0.13379  L
 H-H-0.447800         0    -3.87716  -5.21055  -1.66917  L
 N-N--0.415700        0    -2.1705   -4.34877  -6.28638  L
 C-CT--0.002400      -1    -0.92779  -3.8091   -5.70941  L
 C-C-0.597300         0    -1.04646  -2.27637  -5.66485  L
 O-O--0.567900        0    -1.28816  -1.70013  -6.72664  L
 C-CT--0.034300       0     0.26581  -4.2914   -6.54544  L
 C-CA-0.011800        0     1.61878  -3.75228  -6.11234  L
 C-CA--0.125600       0     2.04525  -3.84038  -4.77048  L
 C-CA--0.125600       0     2.46813  -3.16571  -7.06946  L
 C-CA--0.170400       0     3.28529  -3.29349  -4.38856  L
 C-CA--0.170400       0     3.69804  -2.60903  -6.68575  L
 C-CA--0.107200       0     4.09709  -2.65399  -5.34197  L
 H-H-0.271900         0    -2.36901  -4.20972  -7.27333  L
 H-H1-0.097800        0    -0.78952  -4.20851  -4.70757  L
 H-HC-0.029500        0     0.08999  -4.01647  -7.5871   L
 H-HC-0.029500        0     0.30565  -5.37994  -6.4911   L
 H-HA-0.133000        0     1.42433  -4.32221  -4.02856  L
 H-HA-0.133000        0     2.16883  -3.11749  -8.10347  L
 H-HA-0.143000        0     3.61581  -3.35638  -3.36245  L
 H-HA-0.143000        0     4.323    -2.12649  -7.4233   L
 H-HA-0.129700        0     5.02781  -2.18692  -5.0541   L
 N-N--0.254800        0    -0.94702  -1.63061  -4.48064  L
 C-CT--0.026600       0    -1.13887  -0.18524  -4.32003  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.17722   0.59672  -4.02564  H
 O-O--0.574800        0     0.39096   1.15034  -2.95038  H
 C-CT--0.007000       0    -2.12183  -0.11626  -3.14493  L
 C-CT-0.018900        0    -1.60416  -1.20558  -2.20962  L
 C-CT-0.019200        0    -1.09723  -2.27403  -3.17522  L
 H-H1-0.064100        0    -1.61756   0.25326  -5.19148  L
 H-HC-0.025300        0    -3.12629  -0.36629  -3.4855   L
 H-HC-0.025300        0    -2.13233   0.8505   -2.65506  L
 H-HC-0.021300        0    -2.39517  -1.58723  -1.56293  L
 H-HC-0.021300        0    -0.77577  -0.82485  -1.61596  L
 H-H1-0.039100        0    -0.14838  -2.68177  -2.82809  L
 H-H1-0.039100        0    -1.84627  -3.0609   -3.22273  L
 N-N--0.254800        0     1.13471   0.66363  -4.98993  H
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 C-CT--0.026600       0     2.31958   1.46391  -4.74004  H
 C-C-0.589600         0     2.06898   2.95129  -5.00968  H
 O-O--0.574800        0     1.35135   3.35282  -5.90858  H
 C-CT--0.007000       0     3.32077   0.97491  -5.7993   H
 C-CT-0.018900        0     2.40618   0.63878  -6.97745  H
 C-CT-0.019200        0     1.19819   0.00052  -6.29611  H
 H-H1-0.064100        0     2.67403   1.32703  -3.71463  H
 H-HC-0.025300        0     3.84486   0.09036  -5.42953  H
 H-HC-0.025300        0     4.06549   1.73904  -6.03535  H
 H-HC-0.021300        0     2.86065  -0.03127  -7.70688  H
 H-HC-0.021300        0     2.09675   1.55943  -7.47679  H
 H-H1-0.039100        0     0.29243   0.1448   -6.87725  H
 H-H1-0.039100        0     1.35273  -1.07017  -6.15312  H
 N-N--0.415700        0     2.84639   3.72499  -4.20669  H
 C-CT-0.039700        0     2.92822   5.18022  -4.29936  H
 C-C-0.597300         0     4.03015   5.56914  -5.32827  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.14899   5.06265  -5.205    L
 C-CT--0.003600       0     3.09348   5.62947  -2.84006  H
 C-CT-0.013600        0     3.87995   6.86851  -2.44491  H
 C-C-0.805400         0     4.40836   6.6924   -1.02737  H
 O-O2--0.818800       0     4.63522   5.58735  -0.5152   H
 H-H-0.271900         0     3.03108   3.34005  -3.28905  H
 H-H1-0.110500        0     1.97761   5.54732  -4.68722  H
 H-HC--0.017300       0     2.09349   5.66189  -2.41588  H
 H-HC--0.017300       0     3.54013   4.81686  -2.26416  H
 H-HC--0.042500       0     3.30854   7.80002  -2.50494  H
 H-HC--0.042500       0     4.77837   7.00955  -3.06409  H
 N-N--0.254800        0     3.73801   6.36837  -6.38636  L
 C-CT--0.026600      -1     4.62473   6.60133  -7.54427  L
 C-C-0.589600         0     6.05765   7.06638  -7.23401  L
 O-O--0.574800        0     6.95395   6.88893  -8.05848  L
 C-CT--0.007000       0     3.88705   7.51092  -8.52729  L
 C-CT-0.018900        0     2.60585   7.93148  -7.81436  L
 C-CT-0.019200        0     2.43545   6.96398  -6.64578  L
 H-H1-0.064100        0     4.73362   5.63968  -8.0395   L
 H-HC-0.025300        0     3.63526   6.94211  -9.42343  L
 H-HC-0.025300        0     4.48391   8.37979  -8.8038   L
 H-HC-0.021300        0     1.76009   7.87517  -8.49827  L
 H-HC-0.021300        0     2.70672   8.94477  -7.43005  L
 H-H1-0.039100        0     2.07987   7.5045   -5.76882  L
 H-H1-0.039100        0     1.72242   6.18413  -6.91854  L
 N-N--0.415700        0     6.31595   7.6187   -6.05036  L
 C-CT-0.014300       -1     7.65189   7.85111  -5.51961  L
 C-C-0.597300         0     8.46876   6.57123  -5.38241  L
 O-O--0.567900        0     8.31532   5.79625  -4.43494  L
 C-CT--0.204100       0     7.5401    8.5593   -4.1542   L
 C-C-0.713000         0     8.88991   8.95619  -3.57682  L
 O-O--0.593100        0     9.41107   8.36292  -2.64263  L
 N-N--0.919100        0     9.50028   9.99279  -4.09702  L
 H-H-0.271900         0     5.50843   7.84367  -5.4698   L
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H-H1-0.104800        0     8.17168   8.52242  -6.20553  L
H-HC-0.079700        0     7.03605   7.90523  -3.44442  L
H-HC-0.079700        0     6.94471   9.45512  -4.26677  L
H-H-0.419600         0     10.38064   10.24463  -3.69064  L
H-H-0.419600         0     9.06497   10.56087  -4.82327  L
N-N--0.415700        0     9.43342   6.43498  -6.27955  L
C-CT--0.025200       -1    10.65486   5.71919  -5.992    L
C-C-0.597300         0     11.01184   4.69726  -7.07621  L
O-O--0.567900        0     11.50209   5.04343  -8.14609  L
H-H-0.271900         0     9.38745   7.00815  -7.11104  L
H-H1-0.069800        0     10.59528   5.21271  -5.02814  L
H-H1-0.069800        0     11.47212   6.43798  -5.9367   L
N-N--0.415700        0     10.77652   3.4302   -6.75426  L
C-CT--0.001400       -1    10.80476   2.23421  -7.60833  L
C-C-0.597300         0     9.72996   1.30465  -7.01375  L
O-O--0.567900        0     8.85933   1.7606   -6.26243  L
C-CT--0.015200       0     12.23681   1.65545  -7.62699  L
C-CA--0.001100       0     12.70618   1.24616  -9.00922  L
C-CA--0.190600       0     13.10694   2.24448  -9.91916  L
C-CA--0.190600       0     12.7537  -0.1098   -9.38831  L
C-CA--0.234100       0     13.55898   1.89315  -11.20568  L
C-CA--0.234100       0     13.19495  -0.46461  -10.67776  L
C-C-0.322600         0     13.59971   0.53429  -11.58675  L
O-OH--0.557900       0     14.02234   0.18645  -12.82998  L
H-H-0.271900         0     10.28246   3.29856  -5.88362  L
H-H1-0.087600        0     10.50479   2.50741  -8.62165  L
H-HC-0.029500        0     12.32441   0.81649  -6.93617  L
H-HC-0.029500        0     12.93659   2.4137   -7.27111  L
H-HA-0.169900        0     13.05922   3.2861   -9.62476  L
H-HA-0.169900        0     12.45645  -0.88571  -8.69811  L
H-HA-0.165600        0     13.86264   2.66392  -11.89642  L
H-HA-0.165600        0     13.22905  -1.49867  -10.98518  L
H-HO-0.399200        0     14.29165   0.95385  -13.33456  L
N-N--0.415700        0     9.84362   0.0016   -7.21104  L
C-CT--0.051800       -1    9.40061  -0.98113  -6.22304  L
C-C-0.597300         0     10.58178  -1.87155  -5.88119  L
O-O--0.567900        0     11.5744  -1.94279  -6.6058   L
C-CT--0.110200       0     8.15267  -1.72     -6.75459  L
C-CT-0.353100        0     8.32633  -2.5018   -8.07729  L
C-CT--0.412100       0     8.89367  -3.90885  -7.85893  L
C-CT--0.412100       0     6.96756  -2.66505  -8.75809  L
H-H-0.271900         0     10.52405  -0.30047  -7.89583  L
H-H1-0.092200        0     9.12855  -0.45247  -5.31439  L
H-HC-0.045700        0     7.3837   -0.95957  -6.90028  L
H-HC-0.045700        0     7.78033  -2.39993  -5.98908  L
H-HC--0.036100       0     8.97772  -1.95564  -8.75833  L
H-HC-0.100000        0     9.91871  -3.85412  -7.50136  L
H-HC-0.100000        0     8.89964  -4.44797  -8.80645  L
H-HC-0.100000        0     8.28428  -4.45615  -7.14027  L
H-HC-0.100000        0     6.3      -3.25434  -8.1365   L
H-HC-0.100000        0     7.0925   -3.15548  -9.72458  L
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 H-HC-0.100000        0     6.52305  -1.68788  -8.92932  L
 N-N--0.415700        0     10.49469  -2.51748  -4.73457  L
 C-CT--0.058100       -1    11.58522  -3.29937  -4.17147  L
 C-C-0.597300         0     11.09267  -4.69359  -3.8072   L
 O-O--0.567900        0     9.8967   -4.97559  -3.81191  L
 C-CT--0.007400       0     12.16158  -2.53115  -2.96805  L
 C-CC-0.186800        0     11.14288  -2.17578  -1.90711  L
 N-NB--0.543200       0     10.73467  -2.99926  -0.85822  L
 C-CW--0.220700       0     10.42706  -1.01598  -1.85951  L
 C-CR-0.163500        0     9.79111  -2.31087  -0.19365  L
 N-NA--0.279500       0     9.57263  -1.1256   -0.78356  L
 H-H-0.271900         0     9.63078  -2.42295  -4.21334  L
 H-H1-0.136000        0     12.37663  -3.42414  -4.91275  L
 H-HC-0.036700        0     12.60917  -1.6058   -3.33339  L
 H-HC-0.036700        0     12.95948  -3.11568  -2.51503  L
 H-H4-0.186200        0     10.48505  -0.20382  -2.57101  L
 H-H-0.333900         0     8.83091  -0.4844   -0.5309   L
 H-H5-0.143500        0     9.24477  -2.67167   0.66841  L
 N-N--0.415700        0     12.00891  -5.60139  -3.48856  L
 C-CT--0.059700       -1    11.61952  -6.9742   -3.16487  L
 C-C-0.597300         0     10.69707  -7.09003  -1.92591  L
 O-O--0.567900        0     9.93114  -8.04508  -1.81313  L
 C-CT-0.130300        0     12.85628  -7.88247  -3.05515  L
 C-CT--0.043000       0     12.40089  -9.35348  -2.95567  L
 C-CT--0.320400       0     13.77853  -7.48547  -1.8871   L
 C-CT--0.066000       -1    13.46773  -10.33379  -3.42263  L
 H-H-0.271900         0     12.98557  -5.35373  -3.52045  L
 H-H1-0.086900        0     11.03978  -7.33908  -4.01052  L
 H-HC-0.018700        0     13.41981  -7.76589  -3.98306  L
 H-HC-0.023600        0     11.52922  -9.50994  -3.59197  L
 H-HC-0.023600        0     12.12203  -9.59325  -1.92866  L
 H-HC-0.088200        0     14.68193  -8.09174  -1.91318  L
 H-HC-0.088200        0     13.27946  -7.64096  -0.93004  L
 H-HC-0.088200        0     14.07876  -6.4419   -1.96806  L
 H-HC-0.018600        0     13.07599  -11.34943  -3.35995  L
 H-HC-0.018600        0     14.35247  -10.26    -2.79065  L
 H-HC-0.018600        0     13.74134  -10.12404  -4.45728  L
 N-N--0.415700        0     10.7117  -6.10887  -1.0168   L
 C-CT--0.025200       -1    9.68891  -5.96684   0.02066  L
 C-C-0.597300         0     8.29268  -5.85593  -0.5851   L
 O-O--0.567900        0     7.47513  -6.76496  -0.4303   L
 H-H-0.271900         0     11.33367  -5.32779  -1.16406  L
 H-H1-0.069800        0     9.89518  -5.0881    0.62708  L
 H-H1-0.069800        0     9.71112  -6.84243   0.66491  L
 N-N--0.415700        0     8.04663  -4.77872  -1.34105  L
 C-CT--0.058100       0     6.84999  -4.61594  -2.17937  L    H-HC
246   0.        0.
 C-C-0.597300         0     6.50613  -5.89694  -2.95779  L
 O-O--0.567900        0     5.33631  -6.26713  -3.01523  L
 C-CT--0.007400       0     7.02739  -3.46486  -3.17366  H
 C-CC-0.186800        0     6.96575  -2.03308  -2.74163  H
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N-NB--0.543200       0     7.66151  -1.13184  -3.51148  H
C-CW--0.220700       0     6.17222  -1.36085  -1.84942  H
C-CR-0.163500        0     7.24486   0.05421  -3.13536  H
N-NA--0.279500       0     6.35737  -0.02089  -2.11123  H
H-H-0.271900         0     8.81299  -4.12791  -1.46801  L
H-H1-0.136000        0     5.99071  -4.39527  -1.54321  L
H-HC-0.036700        0     6.25483  -3.60242  -3.93677  H
H-HC-0.036700        0     7.96577  -3.58988  -3.70622  H
H-H4-0.186200        0     5.49086  -1.67166  -1.08131  H
H-H-0.333900         0     5.74608   0.74401  -1.8171   H
H-H5-0.143500        0     7.56158   1.00366  -3.55597  H
N-N--0.415700        0     7.49995  -6.59272  -3.52684  L
C-CT-0.033700       -1     7.3114   -7.85253  -4.25076  L
C-C-0.597300         0     6.51015  -8.91637  -3.49581  L
O-O--0.567900        0     5.68142  -9.58888  -4.10805  L
C-CT--0.182500       0     8.62837  -8.38505  -4.82012  L
H-H-0.271900         0     8.42755  -6.18509  -3.48507  L
H-H1-0.082300        0     6.69715  -7.60253  -5.11358  L
H-HC-0.060300        0     9.17281  -7.58048  -5.31564  L
H-HC-0.060300        0     8.41083  -9.16158  -5.55479  L
H-HC-0.060300        0     9.2332   -8.82629  -4.03332  L
N-N--0.347900        0     6.68248  -9.05086  -2.17624  L
C-CT--0.240000      -1     5.79825  -9.90548  -1.37322  L
C-C-0.734100         0     4.32093  -9.45712  -1.43497  L
O-O--0.589400        0     3.44801  -10.30711  -1.58731  L
C-CT--0.009400       0     6.31401  -10.026    0.07112  L
C-CT-0.018700        0     5.43832  -10.97734   0.91232  L
C-CT--0.047900       0     6.06635  -11.26182   2.28102  L
C-CT--0.014300       0     5.10699  -12.03339   3.19552  L
N-N3--0.385400       0     5.69091  -12.22616   4.5479   L
H-H-0.274700         0     7.36535  -8.44271  -1.72982  L
H-H1-0.142600        0     5.81664  -10.90316  -1.81573  L
H-HC-0.036200        0     6.32928  -9.04094   0.53874  L
H-HC-0.036200        0     7.33474  -10.41126   0.04168  L
H-HC-0.010300        0     5.30706  -11.92108   0.38046  L
H-HC-0.010300        0     4.45977  -10.52068   1.06479  L
H-HC-0.062100        0     6.30689  -10.30819   2.74919  L
H-HC-0.062100        0     6.98065  -11.84003   2.13952  L
H-HP-0.113500        0     4.85568  -12.99496   2.73875  L
H-HP-0.113500        0     4.18527  -11.44809   3.28543  L
H-H-0.340000         0     4.9719   -12.48269   5.22053  L
H-H-0.340000         0     6.04608  -11.33316   4.8899   L
H-H-0.340000         0     6.44182  -12.89815   4.55403  L
N-N--0.415700        0     4.02974  -8.1559   -1.31343  L
C-CT--0.024900      -1     2.67568  -7.58661  -1.49306  L
C-C-0.597300         0     2.12316  -7.86449  -2.90182  L
O-O--0.567900        0     0.99569  -8.3423   -2.99732  L
C-CT-0.211700        0     2.6499   -6.08044  -1.18114  L
O-OH--0.654600       0     1.30535  -5.64993  -1.08344  L
H-H-0.271900         0     4.81646  -7.52113  -1.27621  L
H-H1-0.084300        0     2.00821  -8.07858  -0.78467  L
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H-H1-0.035200        0     3.15962  -5.51844  -1.96384  L
H-H1-0.035200        0     3.15081  -5.90397  -0.22967  L
H-HO-0.427500        0     1.25083  -4.72234  -0.78219  L
N-N--0.415700        0     2.8997   -7.64571  -3.9811   L
C-CT--0.059700       -1    2.56788  -8.08524  -5.36374  L
C-C-0.597300         0     2.15197  -9.57398  -5.32101  L
O-O--0.567900        0     1.02384  -9.89571  -5.67243  L
C-CT-0.130300        0     3.72328  -7.83784  -6.36597  L
C-CT--0.043000       0     4.14117  -6.35344  -6.38545  L
C-CT--0.320400       0     3.30991  -8.27749  -7.78335  L
C-CT--0.066000       0     5.37152  -6.04951  -7.24706  L
H-H-0.271900         0     3.80268  -7.21594  -3.80884  L
H-H1-0.086900        0     1.70042  -7.51661  -5.70106  L
H-HC-0.018700        0     4.58339  -8.43324  -6.06671  L
H-HC-0.023600        0     4.37046  -6.02559  -5.37472  L
H-HC-0.023600        0     3.30749  -5.7587   -6.75024  L
H-HC-0.088200        0     2.49382  -7.65352  -8.14958  L
H-HC-0.088200        0     2.99208  -9.32027  -7.79506  L
H-HC-0.088200        0     4.15253  -8.18863  -8.46852  L
H-HC-0.018600        0     5.1022   -6.04958  -8.30341  L
H-HC-0.018600        0     6.1546   -6.78599  -7.07387  L
H-HC-0.018600        0     5.74964  -5.0655   -6.97803  L
N-N--0.415700        0     3.01984  -10.47914  -4.84836  L
C-CT-0.021300        -1    2.80401  -11.93896  -4.846    L
C-C-0.597300         0     1.5826   -12.4401  -4.07653  L
O-O--0.567900        0     1.0302   -13.47667  -4.429    L
C-CT--0.123100       -1    4.11586  -12.67013  -4.42806  L
S-SH--0.311900       0     5.46001  -12.32939  -5.60116  L
H-H-0.271900         0     3.9254   -10.13732  -4.55104  L
H-H1-0.112400        0     2.60694  -12.22868  -5.88015  L
H-H1-0.111200        0     3.92563  -13.74543  -4.41917  L
H-H1-0.111200        0     4.40684  -12.35603  -3.42492  L
H-HS-0.193300        0     5.61643  -11.03453  -5.28843  L
N-N--0.415700        0     1.1573   -11.73014  -3.03586  L
C-CT--0.051800       -1   -0.07665  -12.0349  -2.31746  L
C-C-0.597300         0    -1.30808  -11.39798  -2.98746  L
O-O--0.567900        0    -2.28368  -12.10508  -3.21238  L
C-CT--0.110200       0     0.06874  -11.55156  -0.8632   L
C-CT-0.353100        0     1.08777  -12.37162  -0.04784  L
C-CT--0.412100       0     1.43369  -11.63354   1.24331  L
C-CT--0.412100       0     0.54748  -13.75265   0.32992  L
H-H-0.271900         0     1.70181  -10.91696  -2.77655  L
H-H1-0.092200        0    -0.24693  -13.11235  -2.31817  L
H-HC-0.045700        0    -0.9026   -11.60908  -0.36961  L
H-HC-0.045700        0     0.374    -10.50347  -0.87511  L
H-HC--0.036100       0     2.00924  -12.50033  -0.61483  L
H-HC-0.100000        0     1.88063  -10.67455   0.98565  L
H-HC-0.100000        0     2.14273  -12.21604   1.82689  L
H-HC-0.100000        0     0.5287   -11.45987   1.82743  L
H-HC-0.100000        0     1.2812   -14.28926   0.92914  L
H-HC-0.100000        0     0.35104  -14.33394  -0.57067  L
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H-HC-0.100000        0    -0.37951  -13.65134   0.89525  L
N-N--0.415700        0    -1.28451  -10.09878  -3.32591  L
C-CT-0.014300       -1    -2.38979  -9.41695   -4.02866  L
C-C-0.597300         0    -2.7476   -10.1161   -5.32575  L
O-O--0.567900        0    -3.89505  -10.51721  -5.52205  L
C-CT--0.204100       0    -2.1325   -7.91123   -4.15133  L
C-C-0.713000         0    -2.3471   -7.21266   -2.8167   L
O-O--0.593100        0    -3.45747  -6.89523   -2.41532  L
N-N--0.919100        0    -1.30075  -6.95044   -2.07413  L
H-H-0.271900         0    -0.42985  -9.58183   -3.15594  L
H-H1-0.104800        0    -3.28146  -9.53112   -3.40695  L
H-HC-0.079700        0    -2.85251  -7.49431   -4.85393  L
H-HC-0.079700        0    -1.13135  -7.71783   -4.53398  L
H-H-0.419600         0    -1.43836  -6.44691   -1.21873  L
H-H-0.419600         0    -0.37957  -7.23597   -2.37882  L
N-N--0.415700        0    -1.73576  -10.34713  -6.15038  L
C-CT--0.002400      -1    -1.87408  -11.18117  -7.32253  L
C-C-0.597300         0    -2.06411  -12.67295  -7.06225  L
O-O--0.567900        0    -2.55401  -13.38786  -7.93057  L
C-CT--0.034300       0    -0.73578  -10.90708  -8.32076  L
C-CA-0.011800        0    -0.87195  -9.5683    -9.03017  L
C-CA--0.125600       0    -1.61216  -9.48569   -10.2255  L
C-CA--0.125600       0    -0.31812  -8.39598   -8.47974  L
C-CA--0.170400       0    -1.81204  -8.24279   -10.85305  L
C-CA--0.170400       0    -0.50765  -7.15412   -9.11437  L
C-CA--0.107200       0    -1.26348  -7.07565   -10.29615  L
H-H-0.271900         0    -0.81286  -10.0058   -5.90881  L
H-H1-0.097800        0    -2.79328  -10.87735  -7.82676  L
H-HC-0.029500        0    -0.74762  -11.6873   -9.08335  L
H-HC-0.029500        0     0.22916  -10.97196  -7.82063  L
H-HA-0.133000        0    -2.0592   -10.37357  -10.64965  L
H-HA-0.133000        0     0.23184  -8.44367   -7.55536  L
H-HA-0.143000        0    -2.41348  -8.17704   -11.75038  L
H-HA-0.143000        0    -0.09625  -6.25262   -8.68897  L
H-HA-0.129700        0    -1.44025  -6.11925   -10.76994  L
N-N--0.415700        0    -1.71952  -13.13498  -5.86649  L
C-CT--0.025200      -1    -1.92645  -14.50335  -5.42352  L
C-C-0.597300         0    -3.38476  -14.92183  -5.27158  L
O-O--0.567900        0    -3.73429  -16.06175  -5.56269  L
H-H-0.271900         0    -1.34471  -12.48109  -5.1986   L
H-H1-0.069800        0    -1.43616  -14.64135  -4.46072  L
H-H1-0.069800        0    -1.45772  -15.17971  -6.13878  L
N-N--0.415700        0    -4.22303  -14.00923  -4.7827   L
C-CT--0.059700      -1    -5.68245  -14.17176  -4.71604  L
C-C-0.597300         0    -6.34721  -14.14708  -6.0958   L
O-O--0.567900        0    -7.36039  -14.81517  -6.29476  L
C-CT-0.130300        0    -6.24339  -13.11749  -3.70509  L
C-CT--0.043000       0    -5.91295  -13.58926  -2.24886  L
C-CT--0.320400      -1    -7.76023  -12.80157  -3.85947  L
C-CT--0.066000      -1    -5.23488  -12.56852  -1.30456  L
H-H-0.271900         0    -3.81506  -13.12385  -4.50752  L
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H-H1-0.086900        0    -5.90232  -15.16376  -4.31939  L
H-HC-0.018700        0    -5.71372  -12.18089  -3.88726  L
H-HC-0.023600        0    -5.24798  -14.45297  -2.28701  L
H-HC-0.023600        0    -6.83086  -13.93593  -1.77237  L
H-HC-0.088200        0    -7.94919  -12.33639  -4.82907  L
H-HC-0.088200        0    -8.07578  -12.10898  -3.07928  L
H-HC-0.088200        0    -8.34262  -13.72092  -3.78857  L
H-HC-0.018600        0    -4.28374  -12.24795  -1.72015  L
H-HC-0.018600        0    -5.06511  -13.02655  -0.33005  L
H-HC-0.018600        0    -5.88296  -11.70006  -1.18622  L
N-N--0.415700        0    -5.75558  -13.42399  -7.04973  L
C-CT--0.149000       -1   -6.15999  -13.43398  -8.44371  L
H-H-0.271900         0    -4.91658  -12.92844  -6.79238  L
H-H1-0.097600        0    -6.43391  -14.44702  -8.74425  L
H-H1-0.097600        0    -5.33771  -13.0842   -9.06905  L
H-H1-0.097600        0    -7.02381  -12.77856  -8.57583  L
C-CT--0.366200       -1   -8.60959  -10.33056  -10.63663  L
C-C-0.597200         0    -7.86023  -9.62965  -9.57004  L
O-O--0.567900        0    -8.20767  -9.64009  -8.39673  L
H-HC-0.112300        0    -7.96699  -11.05232  -11.13515  L
H-HC-0.112300        0    -9.00302  -9.59897  -11.34072  L
H-HC-0.112300        0    -9.44909  -10.84953  -10.17237  L
N-N--0.415700        0    -6.80442  -9.00589  -10.03721  L
C-CT-0.021300        -1   -6.01423  -8.12351  -9.23816  L
C-C-0.597300         0    -5.5241   -6.97332  -10.11667  L
O-O--0.567900        0    -4.91448  -7.23292  -11.15789  L
C-CT--0.123100       0    -4.8092   -8.90033  -8.68525  L
S-SH--0.311900       0    -3.72693  -7.79287  -7.72244  L
H-H-0.271900         0    -6.62322  -9.0309   -11.02772  L
H-H1-0.112400        0    -6.60287  -7.7302   -8.41046  L
H-H1-0.111200        0    -4.24442  -9.32665  -9.51377  L
H-H1-0.111200        0    -5.16666  -9.71561  -8.05589  L
H-HS-0.193300        0    -3.25824  -7.09221  -8.7681   L
N-N--0.415700        0    -5.75133  -5.72443  -9.70665  L
C-CT-0.014300        -1   -5.29666  -4.56496  -10.46968  L
C-C-0.597300         0    -3.92822  -4.00189  -9.9908   L
O-O--0.567900        0    -3.33973  -4.45044  -9.002    L
C-CT--0.204100       0    -6.4307   -3.52618  -10.58354  L
C-C-0.713000         0    -6.25342  -2.56638  -11.75918  L
O-O--0.593100        0    -5.40769  -2.75254  -12.62433  L
N-N--0.919100        0    -6.99107  -1.49325  -11.82554  L
H-H-0.271900         0    -6.28258  -5.5856   -8.85189  L
H-H1-0.104800        0    -5.11481  -4.90657  -11.49039  L
H-HC-0.079700        0    -6.52252  -2.95821  -9.65824  L
H-HC-0.079700        0    -7.36258  -4.05983  -10.75675  L
H-H-0.419600         0    -6.87603  -0.90121  -12.61921  L
H-H-0.419600         0    -7.78748  -1.3626   -11.18588  L
N-N--0.415700        0    -3.392    -3.00731  -10.6995  L
C-CT--0.051800       -1   -2.24496  -2.18264  -10.31934  L
C-C-0.597300         0    -2.75217  -0.73541  -10.08154  L
O-O--0.567900        0    -3.09144  -0.03884  -11.03593  L
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C-CT--0.110200       0    -1.17816  -2.24853  -11.4307  L
C-CT-0.353100        0     0.00863  -1.28398  -11.22564  L
C-CT--0.412100       0     0.82658  -1.63872  -9.98461  L
C-CT--0.412100       0     0.94751  -1.34218  -12.43159  L
H-H-0.271900         0    -3.92094  -2.71044  -11.51646  L
H-H1-0.092200        0    -1.81208  -2.5522   -9.38942  L
H-HC-0.045700        0    -1.65845  -1.99843  -12.37863  L
H-HC-0.045700        0    -0.80602  -3.27122  -11.50259  L
H-HC--0.036100       0    -0.34941  -0.26044  -11.12921  L
H-HC-0.100000        0     1.1743   -2.66737  -10.06455  L
H-HC-0.100000        0     0.21516  -1.52191  -9.08977  L
H-HC-0.100000        0     1.67847  -0.96475  -9.9024   L
H-HC-0.100000        0     1.34719  -2.34946  -12.54851  L
H-HC-0.100000        0     1.76439  -0.63572  -12.29114  L
H-HC-0.100000        0     0.39541  -1.06655  -13.3304  L
N-N--0.347900        0    -2.80143  -0.27469  -8.82266  L
C-CT--0.263700       -1   -3.40523   1.00741  -8.38417  L
C-C-0.734100         0    -2.313     1.97112  -7.95207  L
O-O--0.589400        0    -1.46642   1.60752  -7.14681  L
C-CT--0.000700       0    -4.35597   0.69501  -7.22655  L
C-CT-0.039000        0    -5.22972   1.88997  -6.83593  L
C-CT-0.048600        0    -5.9475    1.59611  -5.51954  L
N-N2--0.529500       0    -5.06716   1.79137  -4.35686  L
C-CA-0.807600        0    -5.46824   1.82065  -3.10632  L
N-N2--0.862700       0    -6.66378   1.48743  -2.75097  L
N-N2--0.862700       0    -4.68081   2.19055  -2.15064  L
H-H-0.274700         0    -2.39214  -0.85722  -8.09862  L
H-H1-0.156000        0    -3.97173   1.44587  -9.20795  L
H-HC-0.032700        0    -3.76469   0.37426  -6.36714  L
H-HC-0.032700        0    -5.01589  -0.12357  -7.52022  L
H-HC-0.028500        0    -5.9707    2.05595  -7.61927  L
H-HC-0.028500        0    -4.6296    2.79394  -6.72104  L
H-H1-0.068700        0    -6.37233   0.59189  -5.53208  L
H-H1-0.068700        0    -6.77328   2.28558  -5.4264   L
H-H-0.345600         0    -4.13272   2.18342  -4.49332  L
H-H-0.447800         0    -6.92627   1.5168   -1.77562  L
H-H-0.447800         0    -7.20368   0.85986  -3.34742  L
H-H-0.447800         0    -5.02087   2.11184  -1.20592  L
H-H-0.447800         0    -3.72978   2.50138  -2.36606  L
N-N--0.415700        0    -2.3138    3.18453  -8.48576  L
C-CT--0.002400       -1   -1.31425   4.17794  -8.1116   L
C-C-0.597300         0    -1.78928   5.02727  -6.92348  L
O-O--0.567900        0    -2.85763   5.62701  -6.97256  L
C-CT--0.034300       0    -0.91483   5.01294  -9.33324  L
C-CA-0.011800        0     0.00328   4.24128  -10.26715  L
C-CA--0.125600       0     1.40063   4.35464  -10.13002  L
C-CA--0.125600       0    -0.53005   3.35429  -11.22237  L
C-CA--0.170400       0     2.25773   3.59633  -10.94865  L
C-CA--0.170400       0     0.32581   2.58812  -12.03378  L
C-CA--0.107200       0     1.72004   2.70902  -11.89837  L
H-H-0.271900         0    -3.06788   3.45555  -9.0938   L
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 H-H1-0.097800        0    -0.40907   3.66499  -7.78302  L
 H-HC-0.029500        0    -0.39137   5.90719  -8.9908   L
 H-HC-0.029500        0    -1.80748   5.3401   -9.86912  L
 H-HA-0.133000        0     1.81235   5.02008  -9.38526  L
 H-HA-0.133000        0    -1.60099   3.24514  -11.32378  L
 H-HA-0.143000        0     3.32667   3.69511  -10.8407  L
 H-HA-0.143000        0    -0.09878   1.90338  -12.75498  L
 H-HA-0.129700        0     2.37171   2.11836  -12.5244  L
 N-N--0.516300        0    -0.9876    5.06834  -5.85586  L
 C-CT-0.038100        0    -1.31216   5.73616  -4.58828  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.58614   7.09271  -4.46803  L
 O-O--0.581900        0     0.30436   7.28033  -3.62947  L
 C-CT--0.030300       0    -0.99842   4.78968  -3.41859  H
 C-C-0.799400         0    -1.99582   3.6529   -3.24777  H
 O-O2--0.801400       0    -2.13807   3.22588  -1.98948  H
 O-O2--0.801400       0    -2.65772   3.11722  -4.10445  H
 H-H-0.293600         0    -0.17957   4.45682  -5.88543  L
 H-H1-0.088000        0    -2.38279   5.94956  -4.55729  L
 H-HC--0.012200       0    -0.99906   5.36345  -2.48657  H
 H-HC--0.012200       0     0.00068   4.3525   -3.53632  H
 N-N--0.516300        0    -0.97961   8.03679  -5.32534  L
 C-CT-0.038100        0    -0.28403   9.28933  -5.67119  L
 C-C-0.536600         0    -0.77621   10.53883  -4.91654  L
 O-O--0.581900        0    -0.45725   11.6688  -5.28711  L
 C-CT--0.030300       0    -0.40951   9.49357  -7.19343  L
 C-C-0.799400         0    -1.79669   9.95977  -7.65529  L
 O-O2--0.801400       0    -2.78895   9.5656   -7.00045  L
 O-O2--0.801400       0    -1.84374   10.65732  -8.69271  L
 H-H-0.293600         0    -1.78866   7.85214  -5.91754  L
 H-H1-0.088000        0     0.77168   9.18126  -5.43486  L
 H-HC--0.012200       0    -0.18863   8.55258  -7.69606  L
 H-HC--0.012200       0     0.33672   10.22583  -7.50775  L
 N-N--0.415700        0    -1.50586   10.34092  -3.81529  L
 C-CT--0.038900      -1    -2.2563    11.35558  -3.04434  L
 C-C-0.597300         0    -1.378     12.55222  -2.53885  L
 O-O--0.567900        0    -1.93537   13.54525  -2.0765   L
 C-CT-0.365400        0    -2.99636   10.72247  -1.8755   L
 O-OH--0.676100       0    -2.15595   9.95533  -1.0329   L
 C-CT--0.243800      -1    -4.04713   9.81762  -2.50102  L
 H-H-0.271900         0    -1.6872    9.37311  -3.59969  L
 H-H1-0.100700        0    -2.99634   11.80036  -3.70965  L
 H-H1-0.004300        0    -3.47937   11.49417  -1.28014  L
 H-HC-0.064200        0    -4.7084    10.40411  -3.13808  L
 H-HC-0.064200        0    -4.6213    9.38571  -1.68864  L
 H-HC-0.064200        0    -3.59709   9.00823  -3.07477  L
 H-HO-0.410200        0    -2.0788    10.44725  -0.18521  L
 N-N--0.415700        0    -0.02926   12.53931  -2.66729  L
 C-CT-0.014300       -1     0.88384   13.71066  -2.54337  L
 C-C-0.597300         0     1.84115   13.79868  -3.75913  L
 O-O--0.567900        0     2.98199   13.33184  -3.65264  L
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C-CT--0.204100       0     1.56276   13.72794  -1.15989  L
C-C-0.713000         0     2.42403   14.96603  -0.94378  L
O-O--0.593100        0     2.72464   15.7425  -1.83881  L
N-N--0.919100        0     2.87643   15.19458   0.2636   L
H-H-0.271900         0     0.29111   11.75426  -3.22092  L
H-H1-0.104800        0     0.26461   14.60617  -2.55747  L
H-HC-0.079700        0     2.17455   12.84336  -1.02867  L
H-HC-0.079700        0     0.78355   13.71697  -0.39547  L
H-H-0.419600         0     3.40236   16.04248   0.3544   L
H-H-0.419600         0     2.61474   14.62215   1.05706  L
N-N--0.254800        0     1.43227   14.44218  -4.87984  L
C-CT--0.026600       -1    2.17539   14.45965  -6.15158  L
C-C-0.589600         0     3.54629   15.11712  -6.0841   L
O-O--0.574800        0     4.39476   14.88191  -6.94081  L
C-CT--0.007000       0     1.24607   15.0947  -7.19069  L
C-CT-0.018900        0     0.25897   15.90143  -6.35339  L
C-CT-0.019200        0     0.13587   15.0824  -5.07141  L
H-H1-0.064100        0     2.33937   13.42396  -6.45071  L
H-HC-0.025300        0     0.70785   14.30522  -7.71884  L
H-HC-0.025300        0     1.78288   15.72462  -7.90134  L
H-HC-0.021300        0    -0.70294   16.01152  -6.85522  L
H-HC-0.021300        0     0.68756   16.87774  -6.12245  L
H-H1-0.039100        0    -0.12123   15.74394  -4.2444   L
H-H1-0.039100        0    -0.63241   14.31673  -5.19467  L
N-N--0.415700        0     3.8216    15.91674  -5.05635  L
C-CT--0.025200       -1    5.00959   16.75813  -5.02041  L
C-C-0.597300         0     6.323     16.09936  -4.60402  L
O-O--0.567900        0     7.21767   16.74357  -4.06255  L
H-H-0.271900         0     3.14039   15.98851  -4.31051  L
H-H1-0.069800        0     4.82448   17.57448  -4.32234  L
H-H1-0.069800        0     5.16243   17.20313  -6.0043   L
N-N--0.347900        0     6.43972   14.81479  -4.90907  L
C-CT--0.240000       -1    7.61472   13.9443  -4.80825  L
C-C-0.734100         0     7.52554   12.84253  -5.9005   L
O-O--0.589400        0     8.27239   11.86404  -5.83113  L
C-CT--0.009400       0     7.66413   13.36404  -3.37277  L
C-CT-0.018700        0     6.4612    12.44052  -3.1471   L
C-CT--0.047900       0     6.30539   11.7637  -1.79324  L
C-CT--0.014300       0     5.27621   10.63234  -1.96773  L
N-N3--0.385400       0     3.8931    11.12509  -2.1757   L
H-H-0.274700         0     5.60248   14.44837  -5.34752  L
H-H1-0.142600        0     8.51757   14.52806  -4.99107  L
H-HC-0.036200        0     7.64533   14.17698  -2.64467  L
H-HC-0.036200        0     8.58679   12.79789  -3.2395   L
H-HC-0.010300        0     6.5645    11.63517  -3.85698  L
H-HC-0.010300        0     5.54494   12.99054  -3.34933  L
H-HC-0.062100        0     5.97641   12.48342  -1.04164  L
H-HC-0.062100        0     7.25944   11.33128  -1.49017  L
H-HP-0.113500        0     5.29899   10.02183  -1.064    L
H-HP-0.113500        0     5.56365   10.00976  -2.81852  L
H-H-0.340000         0     3.33554   10.49008  -2.75708  L
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H-H-0.340000         0     3.85734   11.98244  -2.72545  L
H-H-0.340000         0     3.44523   11.28507  -1.28001  L
N-N--0.516300        0     6.57121   12.93414  -6.84447  L
C-CT-0.039700        -1    6.06091   11.82121  -7.67219  L
C-C-0.536600         0     6.19562   12.11433  -9.19411  L
O-O--0.581900        0     5.90491   13.21805  -9.64397  L
C-CT-0.056000        0     4.65944   11.33511  -7.22266  L
C-CT-0.013600        0     4.71724   11.06748  -5.71139  L
C-C-0.805400         0     3.77994   10.03901  -5.06851  L
O-O2--0.818800       0     2.72586   10.42278  -4.52694  L
O-O2--0.818800       0     4.28087   8.92746  -4.79082  L
H-H-0.293600         0     6.03921   13.79304  -6.94342  L
H-H1-0.110500        0     6.72289   10.97235  -7.50223  L
H-HC--0.017300       0     4.43215   10.41313  -7.75093  L
H-HC--0.017300       0     3.89869   12.08094  -7.4484   L
H-HC--0.042500       0     4.60944   12.02132  -5.19829  L
H-HC--0.042500       0     5.7188    10.69542  -5.51883  L
N-N--0.415700        0     6.72114   11.15344  -9.9848   L
C-CT--0.149000       -1    7.0944    11.30905  -11.40923  L
H-H-0.271900         0     6.91818   10.26684  -9.54822  L
H-H1-0.097600        0     7.84394   12.09622  -11.50729  L
H-H1-0.097600        0     6.21212   11.59815  -11.9843  L
H-H1-0.097600        0     7.49175   10.37282  -11.80237  L
C-CT--0.366200       0     10.16642   1.73725  -12.23296  L
C-C-0.597200         0     9.07716   1.10458  -11.40083  L
O-O--0.567900        0     9.32967   0.72324  -10.2631  L
H-HC-0.112300        0     10.73074   2.4161   -11.59627  L
H-HC-0.112300        0     9.74553   2.29066  -13.06949  L
H-HC-0.112300        0     10.82606   0.95037  -12.59399  L
N-N--0.415700        0     7.86971   1.01026  -11.96609  L
C-CT--0.059700       -1    6.69908   0.37515  -11.33668  L
C-C-0.597300         0     5.95546  -0.52758  -12.33934  L
O-O--0.567900        0     6.17054  -1.73523  -12.33198  L
C-CT-0.130300        0     5.78585   1.40291  -10.60687  L
C-CT--0.043000       0     6.56706   2.15752  -9.49973  L
C-CT--0.320400       0     4.56248   0.70093  -9.98023  L
C-CT--0.066000       0     5.7693    3.22884  -8.74729  L
H-H-0.271900         0     7.79248   1.33286  -12.9162  L
H-H1-0.086900        0     7.07376  -0.30356  -10.57106  L
H-HC-0.018700        0     5.42877   2.13242  -11.33567  L
H-HC-0.023600        0     7.41352   2.67313  -9.95088  L
H-HC-0.023600        0     6.95595   1.43931  -8.77584  L
H-HC-0.088200        0     4.00245   0.13063  -10.71972  L
H-HC-0.088200        0     3.87306   1.43722  -9.5679   L
H-HC-0.088200        0     4.88268   0.02836  -9.18487  L
H-HC-0.018600        0     4.99081   2.77502  -8.13508  L
H-HC-0.018600        0     5.32256   3.92131  -9.4604   L
H-HC-0.018600        0     6.44317   3.78194  -8.09202  L
N-N--0.415700        0     5.08849   0.03311  -13.1966  L
C-CT--0.149000       -1    4.25716  -0.723    -14.13948  L
H-H-0.271900         0     4.95768   1.02979  -13.13196  L
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H-H1-0.097600        0     3.78974  -1.56684  -13.62676  L
H-H1-0.097600        0     4.87666  -1.11178  -14.94957  L
H-H1-0.097600        0     3.47635  -0.08424  -14.55533  L
C-CT--0.366200       -1   -5.13089   16.92011  -3.32174  L
C-C-0.597200         0    -5.67927   16.14603  -2.13551  L
O-O--0.567900        0    -5.48906   16.58388  -1.00425  L
H-HC-0.112300        0    -5.95308   17.3287  -3.90412  L
H-HC-0.112300        0    -4.5199    16.25524  -3.93066  L
H-HC-0.112300        0    -4.50824   17.73163  -2.94942  L
N-N--0.254800        0    -6.41662   15.04803  -2.36982  L
C-CT--0.026600       -1   -7.10191   14.30881  -1.31519  L
C-C-0.589600         0    -6.25623   13.20387  -0.68814  L
O-O--0.574800        0    -5.76853   12.29333  -1.35526  L
C-CT--0.007000       0    -8.32115   13.70871  -2.02611  L
C-CT-0.018900        0    -7.80798   13.41953  -3.43937  L
C-CT-0.019200        0    -6.81079   14.55293  -3.68484  L
H-H1-0.064100        0    -7.44691   14.99193  -0.53828  L
H-HC-0.025300        0    -9.11482   14.45565  -2.07561  L
H-HC-0.025300        0    -8.68617   12.80669  -1.53501  L
H-HC-0.021300        0    -8.61695   13.43027  -4.17019  L
H-HC-0.021300        0    -7.29008   12.46051  -3.46651  L
H-H1-0.039100        0    -5.9464    14.17892  -4.23579  L
H-H1-0.039100        0    -7.30059   15.34896  -4.24652  L
N-N--0.415700        0    -6.16081   13.27832   0.63197  L
C-CT--0.023700       -1   -5.31675   12.44686   1.47726  L
C-C-0.597300         0    -5.51344   10.91754   1.36716  L
O-O--0.567900        0    -6.59924   10.43016   1.04052  L
C-CT-0.034200        0    -5.56914   12.83444   2.9487   L
C-CT-0.001800        0    -5.14301   14.26057   3.32806  L
S-S--0.273700        0    -3.36157   14.54162   3.53308  L
C-CT--0.053600       -1   -3.03465   13.58274   5.04197  L
H-H-0.271900         0    -6.6016    14.07305   1.06141  L
H-H1-0.088000        0    -4.27194   12.65863   1.23689  L
H-HC-0.024100        0    -5.04935   12.1352   3.6037   L
H-HC-0.024100        0    -6.63639   12.73058   3.15138  L
H-H1-0.044000        0    -5.62457   14.51452   4.27249  L
H-H1-0.044000        0    -5.51458   14.95679   2.57643  L
H-H1-0.068400        0    -3.20366   12.52212   4.85223  L
H-H1-0.068400        0    -3.68402   13.91984   5.84893  L
H-H1-0.068400        0    -1.99227   13.71388   5.33234  L
N-N--0.415700        0    -4.46277   10.1708   1.73348  L
C-CT--0.001400       -1   -4.30227   8.72203   1.57578  L
C-C-0.597300         0    -5.52529   7.83249   1.89205  L
O-O--0.567900        0    -6.11257   7.31258   0.94868  L
C-CT--0.015200       0    -3.00029   8.21639   2.21952  L
C-CA--0.001100       0    -2.88053   6.70622   2.35483  L
C-CA--0.190600       0    -3.0488    5.85013   1.24574  L
C-CA--0.190600       0    -2.70309   6.1568    3.63441  L
C-CA--0.234100       0    -3.10077   4.45246   1.439    L
C-CA--0.234100       0    -2.76937   4.76913   3.83199  L
C-C-0.322600         0    -2.98989   3.91233   2.73992  L
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O-OH--0.557900       0    -3.11686   2.57679   2.94889  L
H-H-0.271900         0    -3.60278   10.67707   1.93785  L
H-H1-0.087600        0    -4.15261   8.57789   0.5059   L
H-HC-0.029500        0    -2.91195   8.66701   3.2085   L
H-HC-0.029500        0    -2.16365   8.55652   1.61379  L
H-HA-0.169900        0    -3.22815   6.2742    0.26514  L
H-HA-0.169900        0    -2.59945   6.80934   4.48927  L
H-HA-0.165600        0    -3.31479   3.7897    0.61266  L
H-HA-0.165600        0    -2.72804   4.37499   4.83555  L
H-HO-0.399200        0    -3.45087   2.42801   3.85501  L
N-N--0.516300        0    -5.88182   7.55852   3.15387  L
C-CT-0.038100        -1   -6.83797   6.48898   3.53668  L
C-C-0.536600         0    -8.24815   6.70007   2.98315  L
O-O--0.581900        0    -8.91172   5.73242   2.61803  L
C-CT--0.030300       0    -6.86205   6.30661   5.06632  L
C-C-0.799400         0    -5.58595   5.63843   5.60041  L
O-O2--0.801400       0    -5.47565   4.39507   5.46384  L
O-O2--0.801400       0    -4.71116   6.36195   6.13954  L
H-H-0.293600         0    -5.38243   8.04899   3.89231  L
H-H1-0.088000        0    -6.47256   5.55066   3.12556  L
H-HC--0.012200       0    -7.70834   5.67093   5.3292   L
H-HC--0.012200       0    -7.01841   7.27147   5.55084  L
N-N--0.415700        0    -8.68874   7.95571   2.87342  L
C-CT--0.002400       0    -9.88342   8.33325   2.11661  L
C-C-0.597300         0    -9.78334   7.86578   0.65594  L
O-O--0.567900        0    -10.63128   7.11206   0.17824  L
C-CT--0.034300       0    -10.09388   9.85203   2.21393  L
C-CA-0.011800        0    -11.15442   10.37756   1.26427  L
C-CA--0.125600       0    -12.51963   10.19939   1.55668  L
C-CA--0.125600       0    -10.77352   10.98731   0.05325  L
C-CA--0.170400       0    -13.49866   10.63342   0.64438  L
C-CA--0.170400       0    -11.75154   11.41876  -0.85962  L
C-CA--0.107200       0    -13.11478   11.24252  -0.56383  L
H-H-0.271900         0    -8.03696   8.6734    3.15632  L
H-H1-0.097800        0    -10.74962   7.83454   2.55305  L
H-HC-0.029500        0    -9.15209   10.35912   1.99878  L
H-HC-0.029500        0    -10.37531   10.10458   3.23697  L
H-HA-0.133000        0    -12.81669   9.71      2.4732   L
H-HA-0.133000        0    -9.7255    11.09765  -0.19193  L
H-HA-0.143000        0    -14.54548   10.48222   0.8651   L
H-HA-0.143000        0    -11.44946   11.86663  -1.79572  L
H-HA-0.129700        0    -13.86613   11.5619  -1.27178  L
N-N--0.415700        0    -8.75125   8.3035   -0.06297  L
C-CT--0.038900       -1   -8.57297   7.99047  -1.48537  L
C-C-0.597300         0    -8.39761   6.50827  -1.76687  L
O-O--0.567900        0    -9.04204   5.94835  -2.65139  L
C-CT-0.365400        0    -7.43488   8.82484  -2.08076  L
O-OH--0.676100       0    -7.71176   10.19299  -1.86711  L
C-CT--0.243800       0    -7.2955    8.63503  -3.59184  L
H-H-0.271900         0    -8.07808   8.92747   0.37151  L
H-H1-0.100700        0    -9.48457   8.29316  -2.00043  L
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H-H1-0.004300        0    -6.50954   8.55104  -1.58113  L
H-HC-0.064200        0    -8.2519    8.82687  -4.07855  L
H-HC-0.064200        0    -6.9709    7.61953  -3.81706  L
H-HC-0.064200        0    -6.55711   9.32952  -3.98934  L
H-HO-0.410200        0    -6.8767    10.65545  -1.68814  L
N-N--0.415700        0    -7.55135   5.86967  -0.97115  L
C-CT--0.058100       -1   -7.40358   4.42996  -0.82584  L
C-C-0.597300         0    -8.74446   3.72757  -0.67282  L
O-O--0.567900        0    -9.04888   2.85181  -1.48134  L
C-CT--0.007400       0    -6.45989   4.2223    0.36294  L
C-CC-0.186800        0    -6.35557   2.82268   0.88177  L
N-NB--0.543200       0    -6.45014   1.67266   0.10975  L
C-CW--0.220700       0    -6.23712   2.47907   2.19238  L
C-CR-0.163500        0    -6.43267   0.64619   0.96537  L
N-NA--0.279500       0    -6.28462   1.10598   2.21789  L
H-H-0.271900         0    -7.08935   6.45296  -0.27983  L
H-H1-0.136000        0    -6.93734   4.02727  -1.72431  L
H-HC-0.036700        0    -6.81584   4.83386   1.18434  L
H-HC-0.036700        0    -5.46937   4.57294   0.08175  L
H-H4-0.186200        0    -6.16756   3.15151   3.03967  L
H-H-0.333900         0    -6.27533   0.511     3.04419  L
H-H5-0.143500        0    -6.54946  -0.39317   0.68253  L
N-N--0.415700        0    -9.54874   4.11468   0.32303  L
C-CT-0.021300        -1   -10.84335   3.48361   0.53513  L
C-C-0.597300         0    -11.75656   3.5157   -0.66823  L
O-O--0.567900        0    -12.36781   2.50904  -1.02251  L
C-CT--0.123100       0    -11.50199   3.88513   1.87251  L
S-SH--0.311900       0    -12.59161   5.33489   1.78346  L
H-H-0.271900         0    -9.25141   4.84565   0.96137  L
H-H1-0.112400        0    -10.61736   2.42217   0.64924  L
H-H1-0.111200        0    -10.7319   4.05687   2.62387  L
H-H1-0.111200        0    -12.10392   3.04264   2.21693  L
H-HS-0.193300        0    -11.6816   6.17357   1.26961  L
N-N--0.415700        0    -11.80081   4.67114  -1.31071  L
C-CT--0.059700       -1   -12.6271   4.88017  -2.47207  L
C-C-0.597300         0    -12.15535   4.14654  -3.72838  L
O-O--0.567900        0    -12.97179   3.52042  -4.40035  L
C-CT-0.130300        0    -12.86201   6.4028   -2.66556  L
C-CT--0.043000       0    -14.19802   6.84937  -2.02061  L
C-CT--0.320400       -1   -12.7748   6.89526  -4.11497  L
C-CT--0.066000       -1   -15.48777   6.43367  -2.75956  L
H-H-0.271900         0    -11.26315   5.44059  -0.92626  L
H-H1-0.086900        0    -13.59496   4.43226  -2.24875  L
H-HC-0.018700        0    -12.06972   6.93434  -2.13447  L
H-HC-0.023600        0    -14.19326   7.93749  -1.9427   L
H-HC-0.023600        0    -14.23937   6.45601  -1.00365  L
H-HC-0.088200        0    -11.75672   6.78003  -4.48821  L
H-HC-0.088200        0    -13.02773   7.95466  -4.15902  L
H-HC-0.088200        0    -13.45875   6.33735  -4.75624  L
H-HC-0.018600        0    -16.35236   6.74339  -2.17226  L
H-HC-0.018600        0    -15.52123   5.35213  -2.8903   L
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H-HC-0.018600        0    -15.5392   6.91793  -3.73453  L
N-N--0.415700        0    -10.8674   4.22967  -4.0598   L
C-CT--0.024900       -1   -10.26643   3.51612  -5.19242  L
C-C-0.597300         0    -10.48568   1.99594  -5.01975  L
O-O--0.567900        0    -10.96764   1.35039  -5.94403  L
C-CT-0.211700        0    -8.80996   3.95533  -5.31078  L
O-OH--0.654600       0    -8.31147   3.68427  -6.60368  L
H-H-0.271900         0    -10.26774   4.77396  -3.4481   L
H-H1-0.084300        0    -10.78523   3.81776  -6.10271  L
H-H1-0.035200        0    -8.21243   3.47019  -4.53903  L
H-H1-0.035200        0    -8.75802   5.03418  -5.15611  L
H-HO-0.427500        0    -7.70321   4.38548  -6.85465  L
N-N--0.516300        0    -10.26273   1.43019  -3.81983  L
C-CT-0.038100        -1   -10.56182   0.01439  -3.50916  L
C-C-0.536600         0    -12.04214  -0.37708  -3.63638  L
O-O--0.581900        0    -12.37279  -1.34124  -4.33278  L
C-CT--0.030300       0    -10.00877  -0.39491  -2.12872  L
C-C-0.799400         0    -8.56468  -0.88856  -2.20761  L
O-O2--0.801400       0    -7.94347  -0.77281  -3.28603  L
O-O2--0.801400       0    -8.02761  -1.38712  -1.19323  L
H-H-0.293600         0    -9.90828   2.01635  -3.07181  L
H-H1-0.088000        0    -10.06568  -0.58427  -4.27067  L
H-HC--0.012200       0    -10.61232  -1.20944  -1.72645  L
H-HC--0.012200       0    -10.0839   0.43847  -1.42997  L
N-N--0.415700        0    -12.93147   0.34998  -2.95644  L
C-CT-0.033700        -1   -14.38447   0.20259  -3.05813  L
C-C-0.597300         0    -14.86935   0.20156  -4.52011  L
O-O--0.567900        0    -15.70195  -0.61924  -4.90116  L
C-CT--0.182500       -1   -14.99894   1.36758  -2.34274  L
H-H-0.271900         0    -12.57809   1.11744  -2.3941   L
H-H1-0.082300        0    -14.69526  -0.73186  -2.59024  L
H-HC-0.060300        0    -14.72573   1.33739  -1.28755  L
H-HC-0.060300        0    -16.08569   1.30856  -2.41672  L
H-HC-0.060300        0    -14.66491   2.3114   -2.77264  L
N-N--0.415700        0    -14.37998   1.16509  -5.30719  L
C-CT--0.025200       -1   -14.74973   1.40301  -6.69771  L
C-C-0.597300         0    -14.25996   0.32874  -7.66492  L
O-O--0.567900        0    -15.00501  -0.09553  -8.54338  L
H-H-0.271900         0    -13.70963   1.80323  -4.89006  L
H-H1-0.069800        0    -14.33399   2.35816  -7.01612  L
H-H1-0.069800        0    -15.83558   1.45539  -6.77394  L
N-N--0.516300        0    -13.00455  -0.08547  -7.51191  L
C-CT-0.039700        -1   -12.36592  -1.18016  -8.24676  L
C-C-0.536600         0    -13.08444  -2.52907  -8.05594  L
O-O--0.581900        0    -13.20705  -3.30484  -9.00074  L
C-CT-0.056000        0    -10.89761  -1.22055  -7.79184  L
C-CT-0.013600        0    -10.0136  -2.31183  -8.40584  L
C-C-0.805400         0    -9.57663  -2.04035  -9.84767  L
O-O2--0.818800       0    -9.5752   -2.99266  -10.65973  L
O-O2--0.818800       0    -9.07508  -0.92884  -10.12167  L
H-H-0.293600         0    -12.43717   0.37536  -6.80569  L
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H-H1-0.110500        0    -12.38793  -0.95518  -9.31386  L
H-HC--0.017300       0    -10.89879  -1.36248  -6.71382  L
H-HC--0.017300       0    -10.43849  -0.25128  -7.98748  L
H-HC--0.042500       0    -10.5317   -3.26424  -8.33451  L
H-HC--0.042500       0    -9.10689   -2.38925  -7.80289  L
N-N--0.415700        0    -13.54591  -2.81882  -6.83453  L
C-CT--0.025200       -1   -14.24278  -4.06297  -6.47339  L
C-C-0.597300         0    -13.49179  -4.91032  -5.46176  L
O-O--0.567900        0    -13.82931  -6.08434  -5.29138  L
H-H-0.271900         0    -13.43351  -2.09378  -6.13495  L
H-H1-0.069800        0    -14.41355  -4.67167  -7.36174  L
H-H1-0.069800        0    -15.21208  -3.80821  -6.04669  L
N-N--0.415700        0    -12.4831   -4.34048  -4.7856   L
C-CT--0.059700       -1   -11.74567  -5.03404  -3.72872  L
C-C-0.597300         0    -12.76168  -5.56989  -2.71537  L
O-O--0.567900        0    -13.69139  -4.86877  -2.32198  L
C-CT-0.130300        0    -10.67993  -4.12639  -3.0584   L
C-CT--0.043000       0    -9.3633    -4.08643  -3.85335  L
C-CT--0.320400       0    -10.25802  -4.60403  -1.65167  L
C-CT--0.066000       0    -9.4438    -3.51104  -5.26086  L
H-H-0.271900         0    -12.33113  -3.3472   -4.92575  L
H-H1-0.086900        0    -11.24453  -5.87997  -4.18073  L
H-HC-0.018700        0    -11.07951  -3.11945  -2.96072  L
H-HC-0.023600        0    -8.98449   -5.09641  -3.92523  L
H-HC-0.023600        0    -8.6374    -3.49503  -3.29886  L
H-HC-0.088200        0    -9.50604   -3.9277   -1.24065  L
H-HC-0.088200        0    -9.84697   -5.6132   -1.69884  L
H-HC-0.088200        0    -11.10584  -4.58559  -0.97514  L
H-HC-0.018600        0    -8.44843   -3.49614  -5.70227  L
H-HC-0.018600        0    -9.8217    -2.49634  -5.20768  L
H-HC-0.018600        0    -10.09439  -4.11851  -5.88562  L
N-N--0.415700        0    -12.57485  -6.81813  -2.28432  L
C-CT--0.025200       -1   -13.42686  -7.45504  -1.27205  L
C-C-0.597300         0    -12.87264  -7.37463   0.13348  L
O-O--0.567900        0    -13.5997   -7.16525   1.1024   L
H-H-0.271900         0    -11.83178  -7.3281   -2.74473  L
H-H1-0.069800        0    -13.5552   -8.50572  -1.52736  L
H-H1-0.069800        0    -14.41497  -6.9922   -1.2747   L
N-N--0.415700        0    -11.56343  -7.56149   0.22704  L
C-CT--0.058100       -1   -10.80999  -7.53916   1.46236  L
C-C-0.597300         0    -9.43391   -6.89533   1.18897  L
O-O--0.567900        0    -8.69379   -7.38889   0.33891  L
C-CT--0.007400       0    -10.65804  -8.97771   1.98675  L
C-CC-0.186800        0    -11.95327  -9.5633    2.50197  L
N-NB--0.543200       0    -12.5531   -9.27143   3.73029  L
C-CW--0.220700       0    -12.76784  -10.40333   1.80054  L
C-CR-0.163500        0    -13.72143  -9.92805   3.73336  L
N-NA--0.279500       0    -13.87619  -10.62043   2.59076  L
H-H-0.271900         0    -11.04326  -7.68698  -0.62951  L
H-H1-0.136000        0    -11.33164  -6.94558   2.21484  L
H-HC-0.036700        0    -9.92084   -8.99442   2.78699  L
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H-HC-0.036700        0    -10.27332  -9.61316   1.18756  L
H-H4-0.186200        0    -12.58293  -10.77452   0.80277  L
H-H-0.333900         0    -14.69191  -11.16222   2.34661  L
H-H5-0.143500        0    -14.44124  -9.89196   4.54101  L
N-N--0.415700        0    -9.08911  -5.78285   1.85036  L
C-CT--0.024900       -1   -7.83142  -5.0474    1.60892  L
C-C-0.597300         0    -6.63566  -5.66341   2.33677  L
O-O--0.567900        0    -6.6726   -5.9185    3.54006  L
C-CT-0.211700        0    -7.96428  -3.55114   1.91813  L
O-OH--0.654600       0    -6.68851  -2.92285   1.87547  L
H-H-0.271900         0    -9.70665  -5.47994   2.59566  L
H-H1-0.084300        0    -7.62089  -5.10712   0.5404   L
H-H1-0.035200        0    -8.40621  -3.42481   2.89973  L
H-H1-0.035200        0    -8.62315  -3.08564   1.18265  L
H-HO-0.427500        0    -6.70905  -2.15013   2.47163  L
N-N--0.415700        0    -5.54473  -5.86786   1.59616  L
C-CT--0.051800       -1   -4.24091  -6.25793   2.12823  L
C-C-0.597300         0    -3.36038  -5.03924   2.33694  L
O-O--0.567900        0    -3.14728  -4.27017   1.40114  L
C-CT--0.110200       0    -3.55716  -7.25169   1.16465  L
C-CT-0.353100        0    -4.06629  -8.70577   1.20401  L
C-CT--0.412100       0    -5.44974  -8.89081   0.57984  L
C-CT--0.412100       0    -3.08993  -9.59395   0.42576  L
H-H-0.271900         0    -5.62856  -5.67617   0.60964  L
H-H1-0.092200        0    -4.37354  -6.75152   3.0942   L
H-HC-0.045700        0    -2.5021   -7.27917   1.42699  L
H-HC-0.045700        0    -3.62317  -6.87594   0.1464   L
H-HC--0.036100       0    -4.09136  -9.04916   2.23847  L
H-HC-0.100000        0    -5.4668   -8.48957  -0.43409  L
H-HC-0.100000        0    -6.20477  -8.38577   1.17993  L
H-HC-0.100000        0    -5.70739  -9.94848   0.55098  L
H-HC-0.100000        0    -2.09471  -9.52381   0.86388  L
H-HC-0.100000        0    -3.05159  -9.27839  -0.61745  L
H-HC-0.100000        0    -3.4207   -10.63141   0.47159  L
N-N--0.415700        0    -2.80936  -4.90535   3.53577  L
C-CT-0.021300        -1   -1.8778   -3.83775   3.86705  L
C-C-0.597300         0    -0.73985  -4.3422    4.77263  L
O-O--0.567900        0    -0.73396  -5.50117   5.18991  L
C-CT--0.123100       0    -2.69975  -2.71046   4.50016  L
S-SH--0.311900       0    -1.76801  -1.15881   4.55314  L
H-H-0.271900         0    -3.06333  -5.56061   4.26753  L
H-H1-0.112400        0    -1.41791  -3.45319   2.9535   L
H-H1-0.111200        0    -3.00985  -2.99512   5.50714  L
H-H1-0.111200        0    -3.59071  -2.54329   3.89406  L
H-HS-0.193300        0    -2.68915  -0.47188   5.24481  L
N-N--0.415700        0     0.23793  -3.49707   5.09774  L
C-CT--0.038900       -1    1.35733  -3.85662   5.98024  L
C-C-0.597300         0     1.49183  -2.94231   7.17359  L
O-O--0.567900        0     0.85174  -1.90291   7.30393  L
C-CT-0.365400        0     2.70187  -3.97486   5.23551  L
O-OH--0.676100       0     3.08445  -2.77765   4.59149  L
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C-CT--0.243800       0     2.68869  -5.11472   4.22067  L
H-H-0.271900         0     0.13644  -2.53785   4.78833  L
H-H1-0.100700        0     1.15723  -4.84202   6.40151  L
H-H1-0.004300        0     3.48118  -4.21901   5.95759  L
H-HC-0.064200        0     1.96565  -4.91894   3.43044  L
H-HC-0.064200        0     2.41691  -6.04674   4.71754  L
H-HC-0.064200        0     3.67864  -5.22051   3.78656  L
H-HO-0.410200        0     3.40672  -2.15469   5.28312  L
N-N--0.415700        0     2.32059  -3.4242    8.09068  L
C-CT--0.051800       -1    2.23913  -3.1059    9.49419  L
C-C-0.597300         0     2.33008  -1.60337   9.86168  L
O-O--0.567900        0     1.79351  -1.20782   10.88709  L
C-CT--0.110200       0     3.24448  -3.9696    10.22519  L
C-CT-0.353100        0     2.94745  -4.03208   11.72509  L
C-CT--0.412100       0     1.61262  -4.68827   12.08854  L
C-CT--0.412100       -1    4.05151  -4.90838   12.25432  L
H-H-0.271900         0     2.74845  -4.30348   7.86019  L
H-H1-0.092200        0     1.2376   -3.40886   9.8011   L
H-HC-0.045700        0     4.24118  -3.55827   10.05769  L
H-HC-0.045700        0     3.20436  -4.98268   9.81956  L
H-HC--0.036100       0     3.02821  -3.05033   12.1877  L
H-HC-0.100000        0     1.50303  -5.65173   11.59215  L
H-HC-0.100000        0     0.7857   -4.03939   11.80654  L
H-HC-0.100000        0     1.55099  -4.82643   13.16905  L
H-HC-0.100000        0     3.94489  -4.99058   13.33688  L
H-HC-0.100000        0     5.02366  -4.46192   12.04813  L
H-HC-0.100000        0     3.99508  -5.90834   11.82429  L
N-N--0.516300        0     2.98365  -0.76092   9.05713  L
C-CT-0.039700        -1    3.10508   0.69482   9.29057  L
C-C-0.536600         0     1.83609   1.52558   9.00142  L
O-O--0.581900        0     1.88451   2.75468   9.06654  L
C-CT-0.056000        0     4.32584   1.21975   8.49467  L
C-CT-0.013600        0     4.25555   1.11666   6.95483  L
C-C-0.805400         0     4.83793  -0.18662   6.38318  L
O-O2--0.818800       0     4.21604  -1.26988   6.49959  L
O-O2--0.818800       0     5.97032  -0.1773    5.83403  L
H-H-0.293600         0     3.29611  -1.1264    8.16196  L
H-H1-0.110500        0     3.31237   0.85415   10.34967  L
H-HC--0.017300       0     5.22238   0.70076   8.83838  L
H-HC--0.017300       0     4.46209   2.27109   8.75093  L
H-HC--0.042500       0     4.83189   1.94654   6.54022  L
H-HC--0.042500       0     3.22653   1.24009   6.62643  L
N-N--0.415700        0     0.70944   0.86869   8.71308  L
C-CT--0.002400       -1   -0.60878   1.486     8.52327  L
C-C-0.597300         0    -1.74241   0.81416   9.31413  L
O-O--0.567900        0    -2.92533   1.07989   9.09335  L
C-CT--0.034300       0    -0.97934   1.39396   7.02982  L
C-CA-0.011800        0    -0.02505   1.95462   5.98813  L
C-CA--0.125600       0    -0.14171   3.29606   5.58371  L
C-CA--0.125600       0     0.87672   1.10639   5.31504  L
C-CA--0.170400       0     0.61647   3.77719   4.50266  L
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C-CA--0.170400       0     1.66844   1.59896   4.26004  L
C-CA--0.107200       0     1.5378    2.93751   3.85214  L
H-H-0.271900         0     0.78273  -0.13197   8.57942  L
H-H1-0.097800        0    -0.57488   2.53615   8.8149   L
H-HC-0.029500        0    -1.936     1.89518   6.88561  L
H-HC-0.029500        0    -1.14227   0.3411    6.80508  L
H-HA-0.133000        0    -0.83965   3.95328   6.08418  L
H-HA-0.133000        0     0.95058   0.06844   5.60471  L
H-HA-0.143000        0     0.47734   4.79944   4.18546  L
H-HA-0.143000        0     2.36191   0.94334   3.75329  L
H-HA-0.129700        0     2.14149   3.31713   3.03968  L
N-N--0.415700        0    -1.37272  -0.06545   10.23228  L
C-CT--0.003100      -1    -2.23094  -0.92716   11.02689  L
C-C-0.597300         0    -3.47223  -0.22135   11.63077  L
O-O--0.567900        0    -4.61259  -0.57198   11.3442  L
C-CT--0.003600       0    -1.30283  -1.49201   12.12304  L
C-CT--0.064500       0    -1.9499   -2.21812   13.31489  L
C-C-0.695100         0    -1.01165  -2.2292    14.52063  L
O-O--0.608600        0    -0.53366  -3.26378   14.95764  L
N-N--0.940700        0    -0.70791  -1.09306   15.11665  L
H-H-0.271900         0    -0.37833  -0.10085   10.42034  L
H-H1-0.085000        0    -2.60483  -1.74227   10.42084  L
H-HC-0.017100        0    -0.7251   -0.6561    12.52086  L
H-HC-0.017100        0    -0.59244  -2.17266   11.65561  L
H-HC-0.035200        0    -2.19025  -3.24142   13.02533  L
H-HC-0.035200        0    -2.87004  -1.73036   13.62864  L
H-H-0.425100         0    -0.07028  -1.19122   15.88011  L
H-H-0.425100         0    -0.99259  -0.16865   14.78165  L
N-N--0.516300        0    -3.25667   0.71463   12.54967  L
C-CT-0.038100       -1    -4.24345   1.57259   13.24432  L
C-C-0.536600         0    -4.80311   2.65829   12.32306  L
O-O--0.581900        0    -5.98072   3.00188   12.41938  L
C-CT--0.030300       0    -3.5484    2.19448   14.4715  L
C-C-0.799400         0    -2.09644   2.55597   14.14782  L
O-O2--0.801400       0    -1.87426   3.58842   13.47922  L
O-O2--0.801400       0    -1.22969   1.66763   14.34393  L
H-H-0.293600         0    -2.2792    0.88406   12.76403  L
H-H1-0.088000        0    -5.08548   0.96886   13.58395  L
H-HC--0.012200       0    -3.55589   1.46362   15.28226  L
H-HC--0.012200       0    -4.09456   3.07782   14.80668  L
N-N--0.415700        0    -3.97159   3.16329   11.40499  L
C-CT-0.014300       -1    -4.34216   4.1798    10.42382  L
C-C-0.597300         0    -5.62232   3.83151   9.66467  L
O-O--0.567900        0    -6.43378   4.70603   9.36255  L
C-CT--0.204100       0    -3.20905   4.42399   9.40075  L
C-C-0.713000         0    -1.93474   5.11481   9.86153  L
O-O--0.593100        0    -1.25135   5.72992   9.0559   L
N-N--0.919100        0    -1.50641   5.02817   11.10026  L
H-H-0.271900         0    -3.02551   2.81244   11.42307  L
H-H1-0.104800        0    -4.54071   5.1154    10.9497  L
H-HC-0.079700        0    -3.62088   5.0583    8.61325  L
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H-HC-0.079700        0    -2.93081   3.49485   8.91989  L
H-H-0.419600         0    -0.66739   5.55071   11.26088  L
H-H-0.419600         0    -1.96142   4.54259   11.8762  L
N-N--0.347900        0    -5.79287   2.54158   9.3602   L
C-CT--0.263700       -1   -6.92057   2.01749   8.59798  L
C-C-0.734100         0    -8.3226    2.31652   9.14921  L
O-O--0.589400        0    -9.30627   2.10196   8.44405  L
C-CT--0.000700       0    -6.72167   0.51587   8.3233   L
C-CT-0.039000        0    -7.30879  -0.36919   9.42751  L
C-CT-0.048600        0    -6.89004  -1.82864   9.27327  L
N-N2--0.529500       0    -7.55686  -2.62564   10.30946  L
C-CA-0.807600        0    -7.04404  -2.98174   11.46203  L
N-N2--0.862700       0    -5.77097  -3.0693    11.68421  L
N-N2--0.862700       0    -7.82709  -3.20234   12.46892  L
H-H-0.274700         0    -5.04361   1.91453   9.63252  L
H-H1-0.156000        0    -6.88947   2.52089   7.62964  L
H-HC-0.032700        0    -5.65596   0.3057    8.21538  L
H-HC-0.032700        0    -7.21692   0.26312   7.38426  L
H-HC-0.028500        0    -8.39797  -0.3196    9.39252  L
H-HC-0.028500        0    -6.97595  -0.00443   10.39965  L
H-H1-0.068700        0    -5.80762  -1.88524   9.36323  L
H-H1-0.068700        0    -7.17497  -2.19968   8.29208  L
H-H-0.345600         0    -8.56559  -2.69388   10.26134  L
H-H-0.447800         0    -5.4053   -2.13007   11.79144  L
H-H-0.447800         0    -5.29257  -3.41952   10.84455  L
H-H-0.447800         0    -7.39768  -3.42724   13.34119  L
H-H-0.447800         0    -8.80276  -2.92515   12.36639  L
N-N--0.415700        0    -8.44401   2.78446   10.38843  L
C-CT--0.149000       -1   -9.72401   3.14242   10.97024  L
H-H-0.271900         0    -7.58991   2.93753   10.91239  L
H-H1-0.097600        0    -10.30584   3.74023   10.26763  L
H-H1-0.097600        0    -9.56333   3.71611   11.88373  L
H-H1-0.097600        0    -10.27768   2.23267   11.21137  L
C-CT--0.366200       -1   -9.94841   6.32948   8.74348  L
C-C-0.597200         0    -10.66242   5.57343   7.64755  L
O-O--0.567900        0    -11.84437   5.814     7.44105  L
H-HC-0.112300        0    -9.1376    5.72614   9.15213  L
H-HC-0.112300        0    -10.65904   6.5719    9.53065  L
H-HC-0.112300        0    -9.54021   7.24712   8.32407  L
N-N--0.415700        0    -9.96887   4.65226   6.97505  L
C-CT--0.001400       -1   -10.49048   3.79576   5.88936  L
C-C-0.597300         0    -11.81927   3.09172   6.20104  L
O-O--0.567900        0    -12.69341   2.93908   5.345    L
C-CT--0.015200       0    -9.35001   2.90021   5.35032  L
C-CA--0.001100       0    -9.73369   1.65412   4.57272  L
C-CA--0.190600       0    -10.33938   0.57265   5.24087  L
C-CA--0.190600       0    -9.41788   1.54165   3.20375  L
C-CA--0.234100       0    -10.68147  -0.59114   4.53239  L
C-CA--0.234100       0    -9.71613   0.35821   2.49968  L
C-C-0.322600         0    -10.35912  -0.70404   3.16516  L
O-OH--0.557900       0    -10.68177  -1.83961   2.50192  L
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H-H-0.271900          0    -9.00151   4.53263   7.2351   L
H-H1-0.087600         0    -10.74271   4.46727   5.06697  L
H-HC-0.029500         0    -8.71215   2.5773    6.16556  L
H-HC-0.029500         0    -8.71636   3.52294   4.71745  L
H-HA-0.169900         0    -10.55164   0.64374   6.29828  L
H-HA-0.169900         0    -8.93092   2.36      2.69139  L
H-HA-0.165600         0    -11.17727  -1.40606   5.03144  L
H-HA-0.165600         0    -9.47224   0.25509   1.45075  L
H-HO-0.399200         0    -11.58982  -2.0718    2.76542  L
N-N--0.516300         0    -11.9857   2.68641   7.45246  L
C-CT-0.038100         -1   -13.20998   2.11917   7.99474  L
C-C-0.536600          0    -14.41742   3.07431   8.1458   L
O-O--0.581900         0    -15.5502   2.57518   8.19721  L
C-CT--0.030300        0    -12.87873   1.5648    9.40406  L
C-C-0.799400          0    -12.16906   0.20566   9.40664  L
O-O2--0.801400        0    -12.68644  -0.72368   8.74626  L
O-O2--0.801400        0    -11.15918   0.01527   10.11439  L
H-H-0.293600          0    -11.15684   2.74611   8.03623  L
H-H1-0.088000         0    -13.52738   1.29679   7.3533   L
H-HC--0.012200        0    -13.80709   1.43591   9.96246  L
H-HC--0.012200        0    -12.28515   2.29812   9.9507   L
N-N--0.415700         0    -14.18381   4.38689   8.31857  L
C-CT--0.149000        -1   -15.1381   5.42919   8.72645  L
H-H-0.271900          0    -13.23157   4.69013   8.13022  L
H-H1-0.097600         0    -16.0431   5.35251   8.12165  L
H-H1-0.097600         0    -14.68873   6.41219   8.57507  L
H-H1-0.097600         0    -15.3959   5.30345   9.7784   L
C-CT--0.366200        -1   -19.77613  -1.25508  -1.30866  L
C-C-0.597200          0    -18.77834  -0.88465  -0.1999   L
O-O--0.567900         0    -18.39604   0.2766   -0.13375  L
H-HC-0.112300         0    -20.62788  -1.77438  -0.87642  L
H-HC-0.112300         0    -19.27281  -1.88749  -2.03855  L
H-HC-0.112300         0    -20.1104  -0.34207  -1.79972  L
N-N--0.415700         0    -18.34457  -1.81755   0.6769   L
C-CT--0.058100        -1   -17.21966  -1.58078   1.63161  L
C-C-0.597300          0    -16.36688  -2.80438   1.98041  L
O-O--0.567900         0    -16.7873  -3.6202    2.80563  L
C-CT--0.007400        0    -17.66218  -0.7954    2.87731  L
C-CC-0.186800         0    -16.48156  -0.04934   3.45504  L
N-NB--0.543200        0    -15.43405  -0.64695   4.14735  L
C-CW--0.220700        0    -16.16368   1.26035   3.23292  L
C-CR-0.163500         0    -14.48215   0.29283   4.28579  L
N-NA--0.279500        0    -14.91385   1.46237   3.79027  L
H-H-0.271900          0    -18.69591  -2.75673   0.57958  L
H-H1-0.136000         0    -16.56716  -0.87844   1.11828  L
H-HC-0.036700         0    -18.08158  -1.46943   3.62457  L
H-HC-0.036700         0    -18.42517  -0.06661   2.60206  L
H-H4-0.186200         0    -16.74406   1.96748   2.65404  L
H-H-0.333900          0    -14.35053   2.31116   3.80683  L
H-H5-0.143500         0    -13.51047   0.14105   4.74219  L
N-N--0.254800         0    -15.16268  -2.93273   1.39268  L
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C-CT--0.026600       -1   -14.20356  -3.93973   1.81339  L
C-C-0.589600         0    -13.51453  -3.59259   3.12342  L
O-O--0.574800        0    -13.12646  -2.44662   3.3517   L
C-CT--0.007000       0    -13.15582  -3.98853   0.71     L
C-CT-0.018900        0    -13.19022  -2.60289   0.06765  L
C-CT-0.019200        0    -14.63621  -2.16066   0.26583  L
H-H1-0.064100        0    -14.68915  -4.9125    1.90085  L
H-HC-0.025300        0    -13.47754  -4.73487   0.00018  L
H-HC-0.025300        0    -12.16255  -4.2373    1.08699  L
H-HC-0.021300        0    -12.91913  -2.63326  -0.98805  L
H-HC-0.021300        0    -12.52924  -1.92463   0.60532  L
H-H1-0.039100        0    -14.64875  -1.08863   0.46429  L
H-H1-0.039100        0    -15.21341  -2.38728  -0.63211  L
N-N--0.347900        0    -13.2389  -4.60147   3.95182  L
C-CT--0.263700       -1   -12.47589  -4.40551   5.1913   L
C-C-0.734100         0    -10.96441  -4.74199   5.02093  L
O-O--0.589400        0    -10.63505  -5.60139   4.20926  L
C-CT--0.000700       0    -13.19702  -5.04591   6.39014  L
C-CT-0.039000        0    -14.5192  -4.30169   6.70832  L
C-CT-0.048600        0    -14.31321  -2.91044   7.34763  L
N-N2--0.529500       0    -15.23427  -1.87732   6.81807  L
C-CA-0.807600        0    -15.65123  -0.77458   7.42548  L
N-N2--0.862700       0    -15.36607  -0.49083   8.65584  L
N-N2--0.862700       0    -16.33061   0.13416   6.79439  L
H-H-0.274700         0    -13.50153  -5.53296   3.65546  L
H-H1-0.156000        0    -12.45667  -3.33786   5.40042  L
H-HC-0.032700        0    -12.54983  -5.01696   7.26868  L
H-HC-0.032700        0    -13.41584  -6.08919   6.15899  L
H-HC-0.028500        0    -15.10155  -4.9088    7.40205  L
H-HC-0.028500        0    -15.1074  -4.2037    5.79467  L
H-H1-0.068700        0    -13.29432  -2.57498   7.16     L
H-H1-0.068700        0    -14.42847  -3.00511   8.42889  L
H-H-0.345600         0    -15.42771  -1.89864   5.82182  L
H-H-0.447800         0    -15.60015   0.43405   8.97156  L
H-H-0.447800         0    -14.47498  -0.90185   8.93578  L
H-H-0.447800         0    -16.41369   1.05184   7.21518  L
H-H-0.447800         0    -16.3688   0.036     5.78665  L
N-N--0.415700        0    -10.04179  -4.01879   5.68788  L
C-CT--0.003100       -1   -8.55515  -4.11743   5.56903  L
C-C-0.597300         0    -7.9511   -4.93673   6.71642  L
O-O--0.567900        0    -8.40374  -4.84578   7.85921  L
C-CT--0.003600       0    -7.93207  -2.71519   5.51132  L
C-CT--0.064500       0    -6.39753  -2.78293   5.41791  L
C-C-0.695100         0    -5.81303  -1.46177   4.96759  L
O-O--0.608600        0    -6.05291  -1.04577   3.84674  L
N-N--0.940700        0    -5.0175   -0.7913    5.76624  L
H-H-0.271900         0    -10.38987  -3.32916   6.34416  L
H-H1-0.085000        0    -8.33008  -4.63554   4.64296  L
H-HC-0.017100        0    -8.21603  -2.14337   6.39316  L
H-HC-0.017100        0    -8.32566  -2.19175   4.64217  L
H-HC-0.035200        0    -6.1058   -3.53382   4.68465  L
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H-HC-0.035200        0    -5.98299  -3.06209   6.3841   L
H-H-0.425100         0    -4.74059   0.14437   5.49453  L
H-H-0.425100         0    -4.6894   -1.24333   6.63062  L
N-N--0.415700        0    -6.8936   -5.69115   6.41232  L
C-CT--0.001400       -1   -6.14334  -6.50314   7.36542  L
C-C-0.597300         0    -4.64034  -6.43773   7.07252  L
O-O--0.567900        0    -4.19973  -6.6103    5.92997  L
C-CT--0.015200       0    -6.61833  -7.96821   7.31599  L
C-CA--0.001100       0    -8.11504  -8.16315   7.15608  L
C-CA--0.190600       0    -8.95785  -8.32216   8.27536  L
C-CA--0.190600       0    -8.66494  -8.13397   5.86152  L
C-CA--0.234100       0    -10.35028  -8.46661   8.09492  L
C-CA--0.234100       0    -10.05061  -8.25297   5.68687  L
C-C-0.322600         0    -10.89724  -8.43582   6.79421  L
O-OH--0.557900       0    -12.23047  -8.58684   6.58612  L
H-H-0.271900         0    -6.61155  -5.74104   5.43785  L
H-H1-0.087600        0    -6.31813  -6.11702   8.37083  L
H-HC-0.029500        0    -6.28313  -8.47429   8.22198  L
H-HC-0.029500        0    -6.13258  -8.46456   6.4741   L
H-HA-0.169900        0    -8.53824  -8.31836   9.2708   L
H-HA-0.169900        0    -8.02726  -7.97604   5.00125  L
H-HA-0.165600        0    -11.01259  -8.58946   8.9372   L
H-HA-0.165600        0    -10.47504  -8.17023   4.70434  L
H-HO-0.399200        0    -12.37212  -8.70165   5.63404  L
N-N--0.516300        0    -3.83861  -6.20306   8.10888  L
C-CT-0.039700        -1   -2.38886  -6.11612   7.97824  L
C-C-0.536600         0    -1.68612  -7.48138   8.07127  L
O-O--0.581900        0    -1.89419  -8.25306   9.00728  L
C-CT-0.056000        0    -1.77891  -5.11058   8.9637   L
C-CT-0.013600        0    -2.04241  -3.66167   8.52474  L
C-C-0.805400         0    -3.52271  -3.25195   8.61004  L
O-O2--0.818800       0    -4.22     -3.72475   9.54059  L
O-O2--0.818800       0    -3.96798  -2.45839   7.75169  L
H-H-0.293600         0    -4.25139  -5.8998    8.98288  L
H-H1-0.110500        0    -2.18448  -5.72964   6.98586  L
H-HC--0.017300       0    -0.69669  -5.25334   8.97461  L
H-HC--0.017300       0    -2.15075  -5.28739   9.97395  L
H-HC--0.042500       0    -1.68316  -3.5376    7.50108  L
H-HC--0.042500       0    -1.43911  -3.00678   9.15358  L
N-N--0.415700        0    -0.80276  -7.7693    7.10884  L
C-CT--0.002400       -1   -0.03734  -9.01979   7.01505  L
C-C-0.597300         0     1.46491  -8.77751   7.18518  L
O-O--0.567900        0     1.97777  -7.65365   7.19896  L
C-CT--0.034300       0    -0.38146  -9.71961   5.68072  L
C-CA-0.011800        0     0.17449  -9.04465   4.43433  L
C-CA--0.125600       0    -0.55508  -8.03892   3.77556  L
C-CA--0.125600       0     1.44794  -9.39599   3.95129  L
C-CA--0.170400       0     0.01703  -7.34175   2.69461  L
C-CA--0.170400       0     2.02362  -8.69874   2.87374  L
C-CA--0.107200       0     1.30778  -7.66539   2.24773  L
H-H-0.271900         0    -0.68025  -7.07457   6.37696  L
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H-H1-0.097800        0    -0.35487  -9.67934   7.82357  L
H-HC-0.029500        0    -1.46721  -9.78825   5.59049  L
H-HC-0.029500        0    -0.00475  -10.74213   5.7166   L
H-HA-0.133000        0    -1.53802  -7.76142   4.13265  L
H-HA-0.133000        0     1.98957  -10.19696   4.42401  L
H-HA-0.143000        0    -0.51976  -6.52753   2.22873  L
H-HA-0.143000        0     3.01458  -8.95098   2.52992  L
H-HA-0.129700        0     1.74376  -7.10766   1.43209  L
N-N--0.415700        0     2.20113  -9.87595   7.33707  L
C-CT--0.024900       -1    3.64438  -9.82288   7.52738  L
C-C-0.597300         0     4.39634  -9.34081   6.2698   L
O-O--0.567900        0     4.27218  -9.91215   5.18867  L
C-CT-0.211700        0     4.19045  -11.19334   7.96716  L
O-OH--0.654600       0     3.95061  -12.22799   7.01933  L
H-H-0.271900         0     1.72357  -10.76013   7.28283  L
H-H1-0.084300        0     3.84862  -9.11736   8.33368  L
H-H1-0.035200        0     3.73369  -11.46891   8.91932  L
H-H1-0.035200        0     5.2668   -11.10487   8.1237   L
H-HO-0.427500        0     3.20951  -12.7563   7.34333  L
N-N--0.347900        0     5.24946  -8.32163   6.40621  L
C-CT--0.263700       -1    6.13335  -7.80305   5.33778  L
C-C-0.734100         0     7.22337  -8.79682   4.90087  L
O-O--0.589400        0     7.29047  -9.92929   5.38397  L
C-CT--0.000700       0     6.67462  -6.44042   5.82274  L
C-CT-0.039000        0     7.79278  -6.51414   6.87707  L
C-CT-0.048600        0     8.07163  -5.15282   7.53209  L
N-N2--0.529500       0     8.34639  -4.08008   6.55058  L
C-CA-0.807600        0     7.5538   -3.07247   6.22094  L
N-N2--0.862700       0     6.35644  -2.96288   6.71008  L
N-N2--0.862700       0     7.9332   -2.13552   5.40735  L
H-H-0.274700         0     5.24569  -7.86811   7.30631  L
H-H1-0.156000        0     5.50932  -7.62047   4.46005  L
H-HC-0.032700        0     5.83953  -5.86377   6.22552  L
H-HC-0.032700        0     7.05701  -5.88293   4.97686  L
H-HC-0.028500        0     8.70862  -6.86957   6.40684  L
H-HC-0.028500        0     7.51273  -7.21894   7.66053  L
H-H1-0.068700        0     8.94018  -5.26078   8.18373  L
H-H1-0.068700        0     7.2251   -4.88698   8.16648  L
H-H-0.345600         0     9.26559  -4.08443   6.11524  L
H-H-0.447800         0     5.77208  -2.16263   6.4351   L
H-H-0.447800         0     5.99074  -3.61227   7.36738  L
H-H-0.447800         0     7.25268  -1.38474   5.26726  L
H-H-0.447800         0     8.80682  -2.14677   4.91013  L
N-N--0.415700        0     8.09067  -8.3604    3.9946   L
C-CT--0.051800       -1    9.43074  -8.89824   3.74503  L
C-C-0.597300         0     10.34307  -7.68532   3.91532  L
O-O--0.567900        0     10.36323  -6.77781   3.08758  L
C-CT--0.110200       0     9.45685  -9.54355   2.3441   L
C-CT-0.353100        0     10.79101  -10.1939   1.92397  L
C-CT--0.412100       0     10.52058  -11.27103   0.87067  L
C-CT--0.412100       0     11.77506  -9.20846   1.29579  L
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H-H-0.271900          0     7.90662  -7.44767   3.58388  L
H-H1-0.092200         0     9.68831  -9.65344   4.49017  L
H-HC-0.045700         0     9.15467  -8.81561   1.58993  L
H-HC-0.045700         0     8.70307  -10.32531   2.35514  L
H-HC--0.036100        0     11.25295  -10.6658   2.79136  L
H-HC-0.100000         0     11.45894  -11.74083   0.57397  L
H-HC-0.100000         0     10.05546  -10.82391  -0.01005  L
H-HC-0.100000         0     9.86637  -12.04056   1.27772  L
H-HC-0.100000         0     12.67287  -9.73898   0.98078  L
H-HC-0.100000         0     12.06286  -8.44139   2.00663  L
H-HC-0.100000         0     11.32115  -8.73292   0.42769  L
N-N--0.415700         0     11.03926  -7.62636   5.04333  L
C-CT-0.014300         -1    12.30724  -6.92464   5.07203  L
C-C-0.597300          0     13.36376  -7.97893   4.64811  L
O-O--0.567900         0     13.38479  -9.0464    5.26071  L
C-CT--0.204100        0     12.62756  -6.40072   6.48228  L
C-C-0.713000          0     11.7851  -5.22341   6.93137  L
O-O--0.593100         0     11.09183  -4.55899   6.17638  L
N-N--0.919100         0     11.82066  -4.91575   8.20624  L
H-H-0.271900          0     10.98048  -8.4236    5.65921  L
H-H1-0.104800         0     12.32293  -6.09785   4.36024  L
H-HC-0.079700         0     13.66943  -6.07727   6.49617  L
H-HC-0.079700         0     12.52241  -7.21406   7.20075  L
H-H-0.419600          0     11.31055  -4.0992    8.48418  L
H-H-0.419600          0     12.42612  -5.4263    8.82838  L
N-N--0.415700         0     14.17446  -7.75249   3.60336  L
C-CT--0.051800        -1    15.28318  -8.65929   3.24698  L
C-C-0.597300          0     16.49602  -8.42275   4.18585  L
O-O--0.567900         0     16.75846  -7.27964   4.55645  L
C-CT--0.110200        0     15.65206  -8.52725   1.73509  L
C-CT-0.353100         0     16.67343  -9.5598    1.17131  L
C-CT--0.412100        0     16.18428  -10.99874   1.37313  L
C-CT--0.412100        -1    16.95479  -9.41432  -0.3445   L
H-H-0.271900          0     14.12091  -6.87305   3.11103  L
H-H1-0.092200         0     14.93698  -9.67772   3.41933  L
H-HC-0.045700         0     16.05295  -7.52922   1.56304  L
H-HC-0.045700         0     14.73754  -8.61012   1.14983  L
H-HC--0.036100        0     17.61696  -9.44086   1.69922  L
H-HC-0.100000         0     15.20734  -11.13165   0.9089   L
H-HC-0.100000         0     16.12223  -11.23573   2.4327   L
H-HC-0.100000         0     16.89392  -11.69212   0.92075  L
H-HC-0.100000         0     16.0591  -9.64401  -0.9176   L
H-HC-0.100000         0     17.75748  -10.09209  -0.63533  L
H-HC-0.100000         0     17.27547  -8.39236  -0.55032  L
N-N--0.516300         0     17.22985  -9.47383   4.5849   L
C-CT-0.039700         -1    18.48196  -9.32968   5.36646  L
C-C-0.536600          0     19.56239  -8.52901   4.58231  L
O-O--0.581900         0     19.49226  -8.41307   3.35558  L
C-CT-0.056000         0     19.01939  -10.68784   5.85697  L
C-CT-0.013600         0     18.71447  -10.91741   7.34784  L
C-C-0.805400          0     19.23009  -9.78557   8.25966  L
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O-O2--0.818800       0     18.63537  -9.60802   9.34333  L
O-O2--0.818800       0     20.15619  -9.05474   7.83021  L
H-H-0.293600         0     16.98303  -10.3924   4.26148  L
H-H1-0.110500        0     18.24038  -8.70842   6.22949  L
H-HC--0.017300       0     20.10051  -10.72927   5.71626  L
H-HC--0.017300       0     18.58255  -11.497    5.2689   L
H-HC--0.042500       0     19.16761  -11.86323   7.65292  L
H-HC--0.042500       0     17.63175  -11.01329   7.46196  L
N-N--0.415700        0     20.52554  -7.89869   5.27343  L
C-CT--0.025200       -1    21.52575  -6.96222   4.69911  L
C-C-0.597300         0     20.90077  -5.70031   4.03802  L
O-O--0.567900        0     21.64246  -4.92571   3.43766  L
H-H-0.271900         0     20.54666  -8.10413   6.27688  L
H-H1-0.069800        0     22.10867  -7.48535   3.9412   L
H-H1-0.069800        0     22.20218  -6.63469   5.48773  L
N-N--0.415700        0     19.57305  -5.45986   4.11517  L
C-CT--0.038900       0     18.83404  -4.56757   3.18121  L
C-C-0.597300         0     17.86705  -3.56109   3.84891  L
O-O--0.567900        0     17.04513  -3.90039   4.69792  L
C-CT-0.365400        0     18.03931  -5.40264   2.15469  L
O-OH--0.676100       0     18.81644  -6.42596   1.57451  L
C-CT--0.243800       0     17.55863  -4.56937   0.9649   L
H-H-0.271900         0     19.02087  -6.12323   4.64374  L
H-H1-0.100700        0     19.56728  -3.99426   2.61534  L
H-H1-0.004300        0     17.17198  -5.84357   2.63911  L
H-HC-0.064200        0     16.89221  -3.77598   1.29338  L
H-HC-0.064200        0     17.01589  -5.21403   0.27333  L
H-HC-0.064200        0     18.4147   -4.13699   0.44629  L
H-HO-0.410200        0     19.05524  -7.07649   2.2621   L
N-N--0.415700        0     17.905    -2.2936    3.41185  L
C-CT--0.087500       -1    16.99074  -1.18907   3.80355  L
C-C-0.597300         0     15.6275   -1.34062   3.09049  L
O-O--0.567900        0     15.58258  -1.38057   1.86445  L
C-CT-0.298500        0     17.57927   0.1804    3.38417  L
C-CT--0.319200       -1    16.70527   1.38343   3.84139  L
C-CT--0.319200       -1    19.02488   0.29067   3.90222  L
H-H-0.271900         0     18.5859   -2.09617   2.69375  L
H-H1-0.096900        0     16.84711  -1.20611   4.88317  L
H-HC--0.029700       0     17.6375    0.21937   2.29612  L
H-HC-0.079100        0     16.57954   1.36791   4.92299  L
H-HC-0.079100        0     15.73409   1.36254   3.34751  L
H-HC-0.079100        0     17.2135    2.30411   3.55754  L
H-HC-0.079100        0     19.0523    0.12811   4.97983  L
H-HC-0.079100        0     19.41033   1.28764   3.6863   L
H-HC-0.079100        0     19.678    -0.42766   3.40726  L
N-N--0.415700        0     14.50411  -1.4332    3.82219  L
C-CT--0.023700       -1    13.20535  -1.88876   3.2577   L
C-C-0.597300         0     11.92372  -1.22589   3.84948  L
O-O--0.567900        0     10.80615  -1.72296   3.66804  L
C-CT-0.034200        0     13.09527  -3.41046   3.53781  L
C-CT-0.001800        0     14.17295  -4.33456   2.94759  L
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 S-S--0.273700        0     13.68671  -5.23829   1.45273  L
 C-CT--0.053600       0     13.79874  -3.90697   0.23299  L
 H-H-0.271900         0     14.64483  -1.49118   4.81803  L
 H-H1-0.088000        0     13.18281  -1.72576   2.17974  L
 H-HC-0.024100        0     12.12982  -3.78089   3.1906   L
 H-HC-0.024100        0     13.11539  -3.54333   4.6202   L
 H-H1-0.044000        0     14.42144  -5.07219   3.70977  L
 H-H1-0.044000        0     15.08921  -3.78989   2.74529  L
 H-H1-0.068400        0     14.79746  -3.47054   0.24763  L
 H-H1-0.068400        0     13.06536  -3.13437   0.45804  L
 H-H1-0.068400        0     13.59971  -4.31576  -0.75507  L
 N-N--0.415700        0     12.04944  -0.10144   4.56264  L
 C-CT--0.024900       -1    10.94275   0.84831   4.81813  L
 C-C-0.597300         0     11.05244   1.91251   3.73106  L
 O-O--0.567900        0     12.14924   2.42476   3.50167  L
 C-CT-0.211700        0     11.07043   1.44229   6.22049  L
 O-OH--0.654600       0     10.15456   2.49429   6.44029  L
 H-H-0.271900         0     12.98208   0.28454   4.57591  L
 H-H1-0.084300        0     9.97578   0.35032   4.73268  L
 H-H1-0.035200        0     12.0801   1.82713   6.35316  L
 H-H1-0.035200        0     10.89932   0.65601   6.95692  L
 H-HO-0.427500        0     9.24663   2.18295   6.32775  L
 N-N--0.347900        0     9.9628    2.20144   3.01156  L
 C-CT--0.240000       -1    9.98187   3.12922   1.86846  L
 C-C-0.734100         0     10.54687   4.50209   2.28944  L
 O-O--0.589400        0     11.53794   4.91404   1.6939   L
 C-CT--0.009400       0     8.58054   3.18376   1.23563  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.51496   3.90125  -0.12387  H
 C-CT--0.047900       0     7.17454   3.59547  -0.80477  H
 C-CT--0.014300       0     6.96475   4.37701  -2.09398  H
 N-N3--0.385400       0     5.74196   3.86576  -2.81192  H
 H-H-0.274700         0     9.09033   1.73726   3.25743  L
 H-H1-0.142600        0     10.67201   2.73279   1.12194  L
 H-HC-0.036200        0     7.90326   3.67695   1.92665  L
 H-HC-0.036200        0     8.23255   2.15801   1.09623  L
 H-HC-0.010300        0     9.34181   3.55218  -0.7504   H
 H-HC-0.010300        0     8.63453   4.97159   0.06136  H
 H-HC-0.062100        0     6.32804   3.81693  -0.14639  H
 H-HC-0.062100        0     7.10906   2.52762  -1.0462   H
 H-HP-0.113500        0     7.79481   4.28908  -2.80064  H
 H-HP-0.113500        0     6.78943   5.44084  -1.92008  H
 H-H-0.340000         0     5.99372   3.19194  -3.55122  H
 H-H-0.340000         0     5.27495   4.59333  -3.38613  H
 H-H-0.340000         0     5.04277   3.36382  -2.17336  H
 N-N--0.347900        0     10.06662   5.11869   3.39231  L
 C-CT--0.263700       -1    10.62025   6.34598   4.06356  L
 C-C-0.734100         0     11.90737   6.10936   4.84557  L
 O-O--0.589400        0     12.17177   6.75743   5.8545   L
 C-CT--0.000700       0     9.48184   7.05699   4.8446   L
 C-CT-0.039000        0     8.27487   7.35218   3.91877  L
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C-CT-0.048600        0     7.25622   8.39988   4.39935  L
N-N2--0.529500       0     6.41267   7.9464    5.52042  L
C-CA-0.807600        0     5.24231   8.44401   5.89154  L
N-N2--0.862700       0     4.60493   9.37063   5.23379  L
N-N2--0.862700       0     4.66771   8.00927   6.96964  L
H-H-0.274700         0     9.256     4.67487   3.81131  L
H-H1-0.156000        0     10.9306   7.03528   3.27382  L
H-HC-0.032700        0     9.863     8.00196   5.23507  L
H-HC-0.032700        0     9.15875   6.43785   5.6828   L
H-HC-0.028500        0     7.73846   6.42546   3.7194   L
H-HC-0.028500        0     8.66496   7.71655   2.96735  L
H-H1-0.068700        0     6.61007   8.63245   3.55011  L
H-H1-0.068700        0     7.78463   9.3106    4.68534  L
H-H-0.345600         0     6.72479   7.15886   6.07791  L
H-H-0.447800         0     3.67319   9.64829   5.54888  L
H-H-0.447800         0     4.9152    9.70558   4.34447  L
H-H-0.447800         0     3.7754    8.44262   7.21226  L
H-H-0.447800         0     5.03683   7.24027   7.49679  L
N-N--0.347900        0     12.71533   5.18608   4.31937  L
C-CT--0.240000      -1     14.11725   4.90823   4.63184  L
C-C-0.734100         0     14.97518   4.55518   3.38738  L
O-O--0.589400        0     16.19374   4.59521   3.4977   L
C-CT--0.009400       0     14.26414   3.85964   5.75645  L
C-CT-0.018700        0     13.54967   4.32885   7.03512  L
C-CT--0.047900       0     13.84019   3.52113   8.30049  L
C-CT--0.014300       0     12.99948   4.16668   9.41309  L
N-N3--0.385400       0     13.25624   3.56969   10.74625  L
H-H-0.274700         0     12.32437   4.74947   3.4984   L
H-H1-0.142600        0     14.55716   5.83766   5.00009  L
H-HC-0.036200        0     15.32593   3.73299   5.97451  L
H-HC-0.036200        0     13.86324   2.90082   5.43123  L
H-HC-0.010300        0     12.47304   4.30181   6.86334  L
H-HC-0.010300        0     13.85     5.35911   7.23278  L
H-HC-0.062100        0     14.90463   3.58555   8.53424  L
H-HC-0.062100        0     13.54979   2.48003   8.15368  L
H-HP-0.113500        0     11.94094   4.06697   9.14778  L
H-HP-0.113500        0     13.22626   5.23831   9.43515  L
H-H-0.340000         0     13.02857   2.58465   10.74452  L
H-H-0.340000         0     12.68557   4.0297    11.44579  L
H-H-0.340000         0     14.22858   3.68523   11.00197  L
N-N--0.415700        0     14.38217   4.22183   2.22828  L
C-CT--0.051800      -1     15.04281   3.76137   0.9782   L
C-C-0.597300         0     15.24921   4.84154  -0.05139  L
O-O--0.567900        0     16.21338   4.80704  -0.8131   L
C-CT--0.110200       0     14.20554   2.58074   0.44111  L
C-CT-0.353100        0     14.74866   1.8844   -0.82217  L
C-CT--0.412100       0     16.14707   1.30017  -0.61855  L
C-CT--0.412100       0     13.80948   0.73725  -1.20475  L
H-H-0.271900         0     13.37219   4.23169   2.22215  L
H-H1-0.092200        0     16.03419   3.38676   1.23802  L
H-HC-0.045700        0     13.20073   2.94561   0.22218  L
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H-HC-0.045700        0     14.1213   1.8336    1.23231  L
H-HC--0.036100       0     14.77356   2.59412  -1.64843  L
H-HC-0.100000        0     16.15074   0.61679   0.22952  L
H-HC-0.100000        0     16.86513   2.10119  -0.44559  L
H-HC-0.100000        0     16.45423   0.76075  -1.51417  L
H-HC-0.100000        0     14.16      0.27273  -2.12626  L
H-HC-0.100000        0     12.80309   1.12138  -1.36714  L
H-HC-0.100000        0     13.79028  -0.01201  -0.41204  L
N-N--0.415700        0     14.34887   5.80945  -0.05952  L
C-CT-0.014300       -1     14.54704   7.01961  -0.81127  L
C-C-0.597300         0     15.6248    7.95353  -0.18628  L
O-O--0.567900        0     15.3274    9.05573   0.26702  L
C-CT--0.204100       0     13.17632   7.69646  -1.07549  L
C-C-0.713000         0     12.21278   7.79175   0.10516  L
O-O--0.593100        0     12.55309   7.66655   1.27136  L
N-N--0.919100        0     10.93735   7.96341  -0.16465  L
H-H-0.271900         0     13.60895   5.80035   0.63244  L
H-H1-0.104800        0     14.94245   6.7501   -1.79235  L
H-HC-0.079700        0     12.67252   7.12813  -1.85643  L
H-HC-0.079700        0     13.34287   8.70338  -1.45673  L
H-H-0.419600         0     10.34342   7.95653   0.63983  L
H-H-0.419600         0     10.56981   8.05443  -1.10858  L
N-N--0.415700        0     16.89701   7.51959  -0.21967  L
C-CT--0.149000      -1     18.08704   8.23409   0.26214  L
H-H-0.271900         0     17.01619   6.58223  -0.59022  L
H-H1-0.097600        0     18.01132   8.38266   1.34081  L
H-H1-0.097600        0     18.15024   9.21037  -0.22203  L
H-H1-0.097600        0     18.98635   7.65892   0.03833  L
C-CT--0.055800       0     1.36365   15.06153   4.51527  L
C-CT-0.000000        0     1.42317   14.12582   3.30902  L
O-OS--0.354800       0     2.77199   13.96767   2.86958  L
C-CT--0.202200       0     0.91378   12.72581   3.67581  L
O-OS--0.524600       0     0.18612   12.2616    2.53294  L
C-CT--0.067000       0     2.23851   12.00923   3.92441  L
O-OH--0.613900       0     2.14369   10.61037   3.90094  L
C-CT--0.006600       0     2.96885   12.57338   2.72295  L
N-N*--0.048400       0     4.38528   12.14102   2.62538  L
C-C-0.753800         0     4.76896   11.37071   1.52181  L
O-O--0.625200        0     3.98605   11.10365   0.6107   L
N-NC--0.758400       0     6.04699   10.92212   1.40888  L
C-CA-0.818500        0     6.90495   11.24231   2.3485   L
N-N2--0.953000       0     8.11844   10.8115    2.15459  L
C-CM--0.521500       0     6.57046   11.98094   3.51371  L
C-CM--0.005300       0     5.28954   12.4198    3.61882  L
H-H1-0.067900        0     0.32155   15.19921   4.80605  L
H-H1-0.067900        0     1.9086    14.61701   5.34788  L
H-H1-0.117400        0     0.79596   14.53416   2.51188  L
H-H1-0.061500        0     0.27382   12.75824   4.55741  L
H-H1-0.097200        0     2.68793   12.35423   4.85773  L
H-HO-0.418600        0     1.42821   10.40165   3.27132  L
H-H2-0.202900        0     2.42151   12.23879   1.83999  L
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 H-H-0.423400         0     8.24397   10.34742   1.27499  L
 H-H-0.423400         0     8.86353   11.11166   2.75189  L
 H-HA-0.192800        0     7.28329   12.22357   4.28428  L
 H-H4-0.195800        0     4.96166   13.00498   4.47156  L
 P-P-1.166200         0    -0.8165    10.99329   2.52198  L
 O-O2--0.776000       0    -1.80799   11.13236   1.43362  L
 O-O2--0.776000       0    -1.23701   10.66376   3.8997   L
 O-OS--0.498900       0     0.18568   9.83243   2.08448  L
 C-CT-0.055800        0     0.83623   9.87937   0.83238  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     1.71741   8.6435    0.65708  H
 O-OS--0.354800       0     2.54298   8.50891   1.8067   H
 C-CT-0.202200        0     0.96425   7.32276   0.42278  H
 O-OH--0.654100       0     1.27695   6.76196  -0.83628  H
 C-CT-0.067000        0     1.5431    6.34727   1.48992  H
 O-OH--0.613900       0     2.15541   5.18956   0.98802  H
 C-CT-0.039400        0     2.57051   7.18962   2.27663  H
 N-N*--0.025100       0     2.31494   7.14621   3.70157  H
 C-CK-0.200600        0     1.24853   7.66818   4.41534  H
 N-NB--0.607300       0     1.17517   7.21665   5.64005  H
 C-CB-0.051500        0     2.20664   6.30881   5.73648  H
 C-CA-0.700900        0     2.62149   5.42735   6.75628  H
 N-N2--0.901900       0     2.02698   5.40482   7.98268  H
 N-NC--0.761500       0     3.71129   4.66882   6.54394  H
 C-CQ-0.587500        0     4.24602   4.66113   5.31858  H
 N-NC--0.699700       0     3.95466   5.44172   4.28266  H
 C-CB-0.305300        0     2.92025   6.24557   4.54357  H
 H-H1-0.067900        0     1.45319   10.77283   0.7762   L
 H-H1-0.067900        0     0.10447   9.91953   0.02674  L
 H-H1-0.117400        0     2.34132   8.80023  -0.23094  H
 H-H1-0.061500        0    -0.12031   7.43144   0.5361   H
 H-HO-0.437600        0     0.85226   7.22954  -1.58168  H
 H-H1-0.097200        0     0.7393    6.02744   2.16128  H
 H-HO-0.418600        0     2.51714   5.37946   0.10389  H
 H-H2-0.200700        0     3.55361   6.73983   2.1178   H
 H-H5-0.155300        0     0.57797   8.39906   3.97772  H
 H-H-0.411500         0     2.07614   4.49398   8.45203  H
 H-H-0.411500         0     1.07057   5.75778   8.00223  H
 H-H5-0.047300        0     5.09132   3.99379   5.1716   H
 N-N3-0.149300        0    -0.39732   4.23856  -0.15071  H
 C-CT-0.053600        0     0.25856   3.05741   0.43886  H
 C-CT-0.065100        0    -0.67698   1.83017   0.32983  H
 C-CT--0.090300       0    -0.56643   0.84184   1.49558  H
 C-C-0.735400         0    -1.58911  -0.28196   1.34663  H
 O-O--0.613300        0    -1.2843   -1.43947   1.12365  H
 N-N--1.003100        0    -2.89731   0.13978   1.36701  H
 C-C-0.612300         0     1.55676   2.82016  -0.3222   H
 O-O--0.571300        0     1.81206   3.34003  -1.37643  H
 O-OS--0.421200       0     2.36245   1.93684   0.30679  H
 P-P-1.166200         0     3.95497   1.55293  -0.07174  H
 O-O2--0.776000       0     4.78619   1.74636   1.15072  H
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 O-O2--0.776000       0     4.38109   2.15078  -1.39598  H
 O-OS--0.498900       0     3.79524  -0.0299   -0.30314  H
 C-CT-0.055800        0     3.04615  -0.50861  -1.42364  H
 C-CT-0.106500        0     2.50365  -1.91926  -1.11332  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.50616  -2.83722  -0.67158  L
 C-CT-0.039400        0     3.38027  -3.02467   0.74117  L
 N-N*--0.025100       0     4.71322  -2.92856   1.38906  L
 C-CB-0.305300        0     5.48971  -4.01057   1.72287  L
 N-NC--0.699700       0     5.1535   -5.32348   1.58612  L
 C-CQ-0.587500        0     6.11555  -6.12925   2.00278  L
 N-NC--0.761500       0     7.30308  -5.80731   2.49797  L
 C-CA-0.700900        0     7.60665  -4.51057   2.57613  L
 N-N2--0.901900       0     8.83985  -4.29975   3.00283  L
 C-CB-0.051500        0     6.67325  -3.51195   2.19999  L
 N-NB--0.607300       0     6.66472  -2.10987   2.18984  L
 C-CK-0.200600        0     5.46627  -1.82634   1.73321  L
 C-CT-0.067000        0     2.31238  -2.05819   1.26028  L
 O-OH--0.613900       0     1.5754   -2.57764   2.3541   L
 C-CT-0.202200        0     1.46144  -1.9061   -0.0055   L
 O-OH--0.654100       0     0.57287  -3.00464  -0.17905  L
 H-H-0.199600         0    -1.47664   3.66517  -1.37967  H
 H-H-0.199600         0     0.3002    4.90586  -0.47633  H
 H-H-0.199600         0    -0.96257   4.69992   0.56151  H
 H-HP-0.101500        0     0.53345   3.23195   1.48609  H
 H-HC-0.005000        0    -0.51433   1.3308   -0.63213  H
 H-HC-0.005000        0    -1.70171   2.20585   0.27753  H
 H-HC-0.033100        0    -0.75225   1.37189   2.44013  H
 H-HC-0.033100        0     0.42553   0.3975    1.56686  H
 H-H-0.442900         0    -3.59672  -0.56477   1.54756  H
 H-H-0.442900         0    -3.08052   1.02175   1.85356  H
 H-H1-0.067900        0     3.69418  -0.55974  -2.30546  H
 H-H1-0.067900        0     2.19865   0.1513   -1.65043  H
 H-H1-0.117400        0     2.02977  -2.2911   -2.02102  L
 H-H2-0.200700        0     2.98637  -4.02679   0.92093  L
 H-H5-0.047300        0     5.9032   -7.18596   1.92902  L
 H-H-0.411500         0     9.22533  -3.36788   3.00899  L
 H-H-0.411500         0     9.41979  -5.12988   3.08659  L
 H-H5-0.155300        0     5.11179  -0.81177   1.6008   L
 H-H1-0.097200        0     2.74613  -1.09525   1.52781  L
 H-HO-0.418600        0     2.14061  -2.60299   3.15221  L
 H-H1-0.061500        0     0.91441  -0.96685  -0.0152   L
 H-HO-0.437600        0    -0.18136  -2.77912   0.40641  L
 O-OW--0.834000       0    -10.27171  -2.02198   11.55655  L
 H-HW-0.417000        0    -10.58588  -1.18461   11.13869  L
 H-HW-0.417000        0    -10.55626  -2.68929   10.90715  L
 O-OW--0.834000       0    -10.23834  -3.81705   9.51047  L
 H-HW-0.417000        0    -10.50535  -3.1851    8.8159   L
 H-HW-0.417000        0    -9.60471  -4.38634   9.03284  L
 O-OW--0.834000       0    -10.7104  -1.93585   7.64386  L
 H-HW-0.417000        0    -11.51226  -1.53455   8.06599  L
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H-HW-0.417000        0    -10.07681  -1.21437   7.72242  L
O-OW--0.834000       0     5.47198   4.18348   2.35234  H
H-HW-0.417000        0     4.68459   4.63521   2.71586  H
H-HW-0.417000        0     5.12823   3.42797   1.8317   H
O-OW--0.834000       0     7.30719   3.87215   4.57057  H
H-HW-0.417000        0     7.19322   2.90891   4.47712  H
H-HW-0.417000        0     6.76063   4.17843   3.81909  H
O-OW--0.834000       0     6.57151   2.58906  -5.18457  L
H-HW-0.417000        0     7.35012   2.26372  -5.67813  L
H-HW-0.417000        0     6.29983   3.36964  -5.68878  L
O-OW--0.834000       0     6.69923   5.39941   6.88664  L
H-HW-0.417000        0     5.8855    4.95669   7.17019  L
H-HW-0.417000        0     7.0107    4.83829   6.15465  L
O-OW--0.834000       0     7.30655   1.07337   3.97586  H
H-HW-0.417000        0     6.64905   1.0525    3.25787  H
H-HW-0.417000        0     6.77464   0.63861   4.6973   H
O-OW--0.834000       0     6.79951   6.3394    1.18124  H
H-HW-0.417000        0     6.67481   6.26228   0.2217   H
H-HW-0.417000        0     6.22599   5.60419   1.4926   H
O-OW--0.834000       0     4.58553   15.55352   4.20203  L
H-HW-0.417000        0     3.94998   14.99775   3.72278  L
H-HW-0.417000        0     4.05031   16.28521   4.50993  L
O-OW--0.834000       0    -4.26931   2.12175   5.46282  L
H-HW-0.417000        0    -4.08166   2.09128   6.40557  L
H-HW-0.417000        0    -4.78305   2.9718    5.39363  L
O-OW--0.834000       0     0.09665   1.99832   12.04706  L
H-HW-0.417000        0    -0.22826   1.82696   12.95418  L
H-HW-0.417000        0    -0.10667   2.93125   11.94302  L
O-OW--0.834000       0    -2.37769   9.983     6.17     L
H-HW-0.417000        0    -2.20771   9.03409   6.33467  L
H-HW-0.417000        0    -2.01215   10.13978   5.26684  L
O-OW--0.834000       0     2.23569   9.43952   6.95804  L
H-HW-0.417000        0     1.67946   8.7025    6.64141  L
H-HW-0.417000        0     1.6012    10.18751   6.89061  L
O-OW--0.834000       0    -4.87361   8.98397   5.48657  L
H-HW-0.417000        0    -4.7865    8.08644   5.86503  L
H-HW-0.417000        0    -4.08543   9.44336   5.82232  L
O-OW--0.834000       0    -2.36859   7.32883   6.92715  L
H-HW-0.417000        0    -3.22144   6.89002   6.70384  L
H-HW-0.417000        0    -2.0128    6.78136   7.64112  L
O-OW--0.834000       0     0.15492   11.0663   6.44221  L
H-HW-0.417000        0     0.13977   11.2084   5.48051  L
H-HW-0.417000        0    -0.76657   10.80454   6.61311  L
N-N                  0     4.69986   7.81185  -0.33555  H
H-H                  0     5.25147   7.69215   0.51579  H
H-H                  0     4.6174    8.72951  -0.74283  H
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**TS1**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.7111 | -11.42983 | -5.66284 | L |
| C-C-0.597200 | 0 | -12.01846 | -10.4079 | -6.53456 | L |
| O-O--0.567900 | 0 | -11.62749 | -10.74715 | -7.64255 | L |
| H-HC-0.112300 | 0 | -12.11195 | -11.59977 | -4.77118 | L |
| H-HC-0.112300 | 0 | -12.80152 | -12.35936 | -6.22284 | L |
| H-HC-0.112300 | 0 | -13.70087 | -11.0626 | -5.40066 | L |
| N-N--0.415700 | 0 | -11.83621 | -9.19185 | -6.01067 | L |
| C-CT--0.058100 | -1 | -10.96413 | -8.16233 | -6.59638 | L |
| C-C-0.597300 | 0 | -9.93278 | -7.67048 | -5.5752 | L |
| O-O--0.567900 | 0 | -10.20458 | -7.61737 | -4.36938 | L |
| C-CT--0.007400 | 0 | -11.76044 | -7.04281 | -7.26222 | L |
| C-CC-0.186800 | 0 | -11.15172 | -6.53904 | -8.54515 | L |
| N-NB--0.543200 | 0 | -11.54903 | -6.91436 | -9.82803 | L |
| C-CW--0.220700 | 0 | -10.27146 | -5.50399 | -8.63615 | L |
| C-CR-0.163500 | 0 | -10.9527 | -6.04704 | -10.65918 | L |
| N-NA--0.279500 | 0 | -10.18277 | -5.18754 | -9.97329 | L |
| H-H-0.271900 | 0 | -12.21193 | -8.99876 | -5.09823 | L |
| H-H1-0.136000 | 0 | -10.40048 | -8.64537 | -7.39655 | L |
| H-HC-0.036700 | 0 | -11.82008 | -6.20725 | -6.57439 | L |
| H-HC-0.036700 | 0 | -12.7718 | -7.38591 | -7.48468 | L |
| H-H4-0.186200 | 0 | -9.84262 | -4.95138 | -7.8153 | L |
| H-H-0.333900 | 0 | -9.82378 | -4.30472 | -10.35721 | L |
| H-H5-0.143500 | 0 | -11.13031 | -5.99412 | -11.72391 | L |
| N-N--0.415700 | 0 | -8.73912 | -7.33649 | -6.05972 | L |
| C-CT--0.038900 | -1 | -7.57392 | -6.85538 | -5.29619 | L |
| C-C-0.597300 | 0 | -6.79603 | -5.76749 | -6.07439 | L |
| O-O--0.567900 | 0 | -7.14094 | -5.43766 | -7.20866 | L |
| C-CT-0.365400 | 0 | -6.59412 | -8.00018 | -4.96353 | L |
| O-OH--0.676100 | 0 | -6.32192 | -8.76519 | -6.09891 | L |
| C-CT--0.243800 | -1 | -7.11089 | -8.95577 | -3.90522 | L |
| H-H-0.271900 | 0 | -8.59038 | -7.5176 | -7.04656 | L |
| H-H1-0.100700 | 0 | -7.89221 | -6.43844 | -4.34852 | L |
| H-H1-0.004300 | 0 | -5.65855 | -7.58345 | -4.59042 | L |
| H-HC-0.064200 | 0 | -7.37649 | -8.40144 | -3.00498 | L |
| H-HC-0.064200 | 0 | -6.33799 | -9.68238 | -3.65962 | L |
| H-HC-0.064200 | 0 | -7.99299 | -9.47794 | -4.27682 | L |
| H-HO-0.410200 | 0 | -5.61497 | -9.40095 | -5.90191 | L |
| N-N--0.347900 | 0 | -5.71609 | -5.20394 | -5.49818 | L |
| C-CT--0.263700 | -1 | -4.72182 | -4.35588 | -6.20595 | L |
| C-C-0.734100 | 0 | -3.31767 | -4.45696 | -5.62311 | L |
| O-O--0.589400 | 0 | -3.19426 | -4.72374 | -4.43394 | L |
| C-CT--0.000700 | 0 | -5.19631 | -2.89353 | -6.29411 | L |
| C-CT-0.039000 | 0 | -4.95714 | -2.01813 | -5.05219 | L |
| C-CT-0.048600 | 0 | -5.77322 | -2.36313 | -3.8073 | L |
| N-N2--0.529500 | 0 | -5.17554 | -3.42891 | -2.99763 | L |
| C-CA-0.807600 | 0 | -5.1746 | -3.51974 | -1.68767 | L |
| N-N2--0.862700 | 0 | -5.87351 | -2.75601 | -0.90209 | L |
| N-N2--0.862700 | 0 | -4.41803 | -4.42014 | -1.14615 | L |
| H-H-0.274700 | 0 | -5.48799 | -5.52194 | -4.5684 | L |
| H-H1-0.156000 | 0 | -4.67245 | -4.74594 | -7.21912 | L |

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 H-HC-0.032700        0    -6.25532  -2.86491  -6.55569  L
 H-HC-0.032700        0    -4.65842  -2.42694  -7.12064  L
 H-HC-0.028500        0    -5.2381   -1.01034  -5.32556  L
 H-HC-0.028500        0    -3.89944  -1.98861  -4.80404  L
 H-H1-0.068700        0    -6.78095  -2.64056  -4.1116   L
 H-H1-0.068700        0    -5.81726  -1.45805  -3.19995  L
 H-H-0.345600         0    -4.52673  -4.04647  -3.46246  L
 H-H-0.447800         0    -5.91238  -2.88685   0.09786  L
 H-H-0.447800         0    -6.61585  -2.16172  -1.29603  L
 H-H-0.447800         0    -4.1329   -4.28237  -0.1828   L
 H-H-0.447800         0    -3.97274  -5.12097  -1.73021  L
 N-N--0.415700        0    -2.26934  -4.13098  -6.37349  L
 C-CT--0.002400      -1    -1.02083  -3.62963  -5.77349  L
 C-C-0.597300         0    -1.08003  -2.09484  -5.71242  L
 O-O--0.567900        0    -1.14659  -1.48128  -6.78117  L
 C-CT--0.034300       0     0.19362  -4.11574  -6.57197  L
 C-CA-0.011800        0     1.50933  -3.5473   -6.06665  L
 C-CA--0.125600       0     1.98538  -3.87127  -4.77982  L
 C-CA--0.125600       0     2.25578  -2.67659  -6.88189  L
 C-CA--0.170400       0     3.19014  -3.31134  -4.31386  L
 C-CA--0.170400       0     3.45838  -2.12043  -6.41716  L
 C-CA--0.107200       0     3.91492  -2.421    -5.12555  L
 H-H-0.271900         0    -2.46712  -3.95339  -7.35418  L
 H-H1-0.097800        0    -0.90657  -4.03165  -4.76856  L
 H-HC-0.029500        0     0.06082  -3.84278  -7.62033  L
 H-HC-0.029500        0     0.23983  -5.20376  -6.51157  L
 H-HA-0.133000        0     1.42557  -4.54488  -4.14592  L
 H-HA-0.133000        0     1.90167  -2.42231  -7.86755  L
 H-HA-0.143000        0     3.55873  -3.5578   -3.32942  L
 H-HA-0.143000        0     4.02348  -1.44828  -7.04711  L
 H-HA-0.129700        0     4.82156  -1.95601  -4.76633  L
 N-N--0.254800        0    -1.1085   -1.47886  -4.51105  L
 C-CT--0.026600       0    -1.19514  -0.03197  -4.35512  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.15113   0.59612  -3.9148   H
 O-O--0.574800        0     0.57345   0.43341  -2.78015  H
 C-CT--0.007000       0    -2.26435   0.14463  -3.27433  L
 C-CT-0.018900        0    -2.03016  -1.03793  -2.3315   L
 C-CT-0.019200        0    -1.40021  -2.11033  -3.22397  L
 H-H1-0.064100        0    -1.54337   0.42713  -5.26628  L
 H-HC-0.025300        0    -3.25479   0.07035  -3.72307  L
 H-HC-0.025300        0    -2.16206   1.09032  -2.75127  L
 H-HC-0.021300        0    -2.96767  -1.38102  -1.89309  L
 H-HC-0.021300        0    -1.33201  -0.76115  -1.54378  L
 H-H1-0.039100        0    -0.48419  -2.48683  -2.76804  L
 H-H1-0.039100        0    -2.11624  -2.91733  -3.3371   L
 N-N--0.254800        0     0.83816   1.38528  -4.79759  H
 C-CT--0.026600       0     2.08708   1.9916   -4.36928  H
 C-C-0.589600         0     2.11313   3.50678  -4.6032   H
 O-O--0.574800        0     1.55369   4.02539  -5.5566   H
 C-CT--0.007000       0     3.10748   1.38577  -5.34914  H
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 C-CT-0.018900        0     2.33252   1.32647  -6.67451  H
 C-CT-0.019200        0     0.83964   1.28608  -6.26516  H
 H-H1-0.064100        0     2.28444   1.76596  -3.32267  H
 H-HC-0.025300        0     3.39373   0.39324  -4.99497  H
 H-HC-0.025300        0     4.00599   2.00223  -5.42444  H
 H-HC-0.021300        0     2.61341   0.46722  -7.28371  H
 H-HC-0.021300        0     2.51718   2.23004  -7.25779  H
 H-H1-0.039100        0     0.33585   2.14579  -6.6968   H
 H-H1-0.039100        0     0.3475    0.37139  -6.58853  H
 N-N--0.415700        0     2.95539   4.11298  -3.70644  H
 C-CT-0.039700        0     3.4228    5.49366  -3.79694  H
 C-C-0.597300         0     4.27012   5.65482  -5.10978  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.30702   4.98886  -5.20493  L
 C-CT--0.003600       0     4.1338    5.72017  -2.42782  H
 C-CT-0.013600        0     5.17031   6.82026  -2.31905  H
 C-C-0.805400         0     6.0489    6.72686  -1.07679  H
 O-O2--0.818800       0     6.1537    5.74733  -0.33598  H
 H-H-0.271900         0     2.82155   3.7694   -2.75127  H
 H-H1-0.110500        0     2.59098   6.20381  -3.86385  H
 H-HC--0.017300       0     3.3418    5.85725  -1.69106  H
 H-HC--0.017300       0     4.59671   4.79513  -2.07733  H
 H-HC--0.042500       0     4.72486   7.81993  -2.33225  H
 H-HC--0.042500       0     5.85833   6.77141  -3.16999  H
 N-N--0.254800        0     3.87325   6.46394  -6.14021  L
 C-CT--0.026600       -1    4.66651   6.74717  -7.37053  L
 C-C-0.589600         0     6.10294   7.20512  -7.05177  L
 O-O--0.574800        0     6.99969   7.03415  -7.87782  L
 C-CT--0.007000       0     3.87401   7.71367  -8.24404  L
 C-CT-0.018900        0     2.60162   8.03172  -7.46289  L
 C-CT-0.019200        0     2.58036   7.13105  -6.22698  L
 H-H1-0.064100        0     4.75064   5.81242  -7.91881  L
 H-HC-0.025300        0     3.61579   7.22545  -9.18473  L
 H-HC-0.025300        0     4.44328   8.61747  -8.45262  L
 H-HC-0.021300        0     1.73218   7.83088  -8.08729  L
 H-HC-0.021300        0     2.60525   9.07737  -7.15667  L
 H-H1-0.039100        0     2.39029   7.73557  -5.34076  L
 H-H1-0.039100        0     1.78622   6.39324  -6.33659  L
 N-N--0.415700        0     6.36585   7.73072  -5.84807  L
 C-CT-0.014300        -1    7.71328   7.90811  -5.32253  L
 C-C-0.597300         0     8.50539   6.61543  -5.13865  L
 O-O--0.567900        0     8.38477   5.90122  -4.14138  L
 C-CT--0.204100       0     7.75881   8.8159   -4.0805   L
 C-C-0.713000         0     9.16906   9.05612  -3.55939  L
 O-O--0.593100        0     9.66557   8.39861  -2.65618  L
 N-N--0.919100        0     9.86344   10.02551  -4.10024  L
 H-H-0.271900         0     5.56838   7.97022  -5.25917  L
 H-H1-0.104800        0     8.2441    8.47514  -6.08997  L
 H-HC-0.079700        0     7.17299   8.39405  -3.28593  L
 H-HC-0.079700        0     7.32942   9.77381  -4.33345  L
 H-H-0.419600         0     10.77183   10.19819  -3.7155   L
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H-H-0.419600         0     9.42563   10.65685  -4.76965  L
N-N--0.415700        0     9.42149   6.41551  -6.08007  L
C-CT--0.025200       -1    10.68689   5.7485   -5.8514   L
C-C-0.597300         0     11.02736   4.77111  -6.98333  L
O-O--0.567900        0     11.46296   5.15651  -8.06294  L
H-H-0.271900         0     9.31527   6.94786  -6.93406  L
H-H1-0.069800        0     10.67165   5.21453  -4.90057  L
H-H1-0.069800        0     11.47697   6.49783  -5.80602  L
N-N--0.415700        0     10.81727   3.49464  -6.69072  L
C-CT--0.001400       -1    10.78786   2.30138  -7.55061  L
C-C-0.597300         0     9.78575   1.37182  -6.85672  L
O-O--0.567900        0     9.09506   1.79411  -5.91961  L
C-CT--0.015200       0     12.21508   1.71748  -7.64074  L
C-CA--0.001100       0     12.64799   1.34777  -9.04456  L
C-CA--0.190600       0     13.10045   2.36058  -9.91297  L
C-CA--0.190600       0     12.62667   0.00715  -9.47667  L
C-CA--0.234100       0     13.54005   2.03748  -11.2113  L
C-CA--0.234100       0     13.05438  -0.31829  -10.77835  L
C-C-0.322600         0     13.5149   0.69398  -11.64529  L
O-OH--0.557900       0     13.92438   0.37453  -12.90044  L
H-H-0.271900         0     10.3862   3.34031  -5.79027  L
H-H1-0.087600        0     10.4189   2.56426  -8.54347  L
H-HC-0.029500        0     12.31434   0.85108  -6.98561  L
H-HC-0.029500        0     12.93238   2.45386  -7.27369  L
H-HA-0.169900        0     13.10495   3.39048  -9.57661  L
H-HA-0.169900        0     12.28907  -0.77853  -8.81533  L
H-HA-0.165600        0     13.88525   2.81834  -11.87052  L
H-HA-0.165600        0     13.03783  -1.34003  -11.12597  L
H-HO-0.399200        0     14.2405   1.14528  -13.37172  L
N-N--0.415700        0     9.76609   0.09413  -7.19284  L
C-CT--0.051800       -1    9.34337  -0.92721  -6.23959  L
C-C-0.597300         0     10.50072  -1.86678  -5.95062  L
O-O--0.567900        0     11.46424  -1.96768  -6.7092   L
C-CT--0.110200       0     8.05143  -1.60327  -6.74644  L
C-CT-0.353100        0     8.1373   -2.34262  -8.09959  L
C-CT--0.412100       0     8.65602  -3.7764   -7.95017  L
C-CT--0.412100       0     6.74106  -2.41898  -8.7175   L
H-H-0.271900         0     10.29755  -0.18839  -8.00672  L
H-H1-0.092200        0     9.1116   -0.44677  -5.29494  L
H-HC-0.045700        0     7.303    -0.81344  -6.82994  L
H-HC-0.045700        0     7.68703  -2.29869  -5.99139  L
H-HC--0.036100       0     8.78187  -1.79879  -8.78916  L
H-HC-0.100000        0     9.69387  -3.77189  -7.626    L
H-HC-0.100000        0     8.6087   -4.28125  -8.91521  L
H-HC-0.100000        0     8.05083  -4.32544  -7.22946  L
H-HC-0.100000        0     6.05831  -2.94535  -8.05547  L
H-HC-0.100000        0     6.78532  -2.92807  -9.6814   L
H-HC-0.100000        0     6.36219  -1.41418  -8.88091  L
N-N--0.415700        0     10.42389  -2.5124   -4.80005  L
C-CT--0.058100       -1    11.50033  -3.32245  -4.24808  L
C-C-0.597300         0     10.9911  -4.71872  -3.91536  L
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 O-O--0.567900        0     9.79269  -4.98781  -3.92877  L
 C-CT--0.007400       0     12.08984  -2.58501  -3.03174  L
 C-CC-0.186800        0     11.0839  -2.24524  -1.95343  L
 N-NB--0.543200       0     10.64711  -3.10449  -0.94583  L
 C-CW--0.220700       0     10.41335  -1.06262  -1.84363  L
 C-CR-0.163500        0     9.72798  -2.41787  -0.24616  L
 N-NA--0.279500       0     9.55579  -1.19547  -0.77191  L
 H-H-0.271900         0     9.57567  -2.38786  -4.25874  L
 H-H1-0.136000        0     12.28926  -3.44091  -4.99305  L
 H-HC-0.036700        0     12.54244  -1.65556  -3.38008  L
 H-HC-0.036700        0     12.88676  -3.18549  -2.59867  L
 H-H4-0.186200        0     10.5032  -0.21808  -2.51263  L
 H-H-0.333900         0     8.83731  -0.5442   -0.4809   L
 H-H5-0.143500        0     9.16581  -2.80329   0.59525  L
 N-N--0.415700        0     11.89576  -5.64505  -3.61802  L
 C-CT--0.059700       -1    11.48744  -7.02038  -3.3294   L
 C-C-0.597300         0     10.56671  -7.15494  -2.09103  L
 O-O--0.567900        0     9.79029  -8.10373  -1.99917  L
 C-CT-0.130300        0     12.71195  -7.94766  -3.2449   L
 C-CT--0.043000       0     12.2366  -9.41422  -3.18092  L
 C-CT--0.320400       0     13.64161  -7.59264  -2.06919  L
 C-CT--0.066000       -1    13.29044  -10.39704  -3.67071  L
 H-H-0.271900         0     12.87548  -5.40931  -3.64252  L
 H-H1-0.086900        0     10.90114  -7.35567  -4.18271  L
 H-HC-0.018700        0     13.27538  -7.81572  -4.1708   L
 H-HC-0.023600        0     11.3633  -9.54349  -3.82107  L
 H-HC-0.023600        0     11.95419  -9.67501  -2.16004  L
 H-HC-0.088200        0     14.53702  -8.2096   -2.11268  L
 H-HC-0.088200        0     13.14232  -7.76607  -1.11529  L
 H-HC-0.088200        0     13.95521  -6.55132  -2.12392  L
 H-HC-0.018600        0     12.88477  -11.40845  -3.63341  L
 H-HC-0.018600        0     14.17527  -10.35105  -3.03625  L
 H-HC-0.018600        0     13.56824  -10.16572  -4.69963  L
 N-N--0.415700        0     10.59537  -6.19596  -1.15876  L
 C-CT--0.025200       -1    9.57555  -6.06381  -0.11704  L
 C-C-0.597300         0     8.18005  -5.92705  -0.72065  L
 O-O--0.567900        0     7.35566  -6.83323  -0.58868  L
 H-H-0.271900         0     11.22466  -5.41805  -1.29086  L
 H-H1-0.069800        0     9.79127  -5.20024   0.50745  L
 H-H1-0.069800        0     9.58862  -6.9534    0.50788  L
 N-N--0.415700        0     7.94218  -4.83167  -1.45257  L
 C-CT--0.058100       0     6.74524  -4.63884  -2.28498  L    H-HC
246   0.        0.
 C-C-0.597300         0     6.38356  -5.89361  -3.08843  L
 O-O--0.567900        0     5.20884  -6.24533  -3.15926  L
 C-CT--0.007400       0     6.93946  -3.48192  -3.2656   H
 C-CC-0.186800        0     6.92464  -2.0687   -2.78762  H
 N-NB--0.543200       0     7.66918  -1.16065  -3.49642  H
 C-CW--0.220700       0     6.12369  -1.41314  -1.88932  H
 C-CR-0.163500        0     7.27568   0.02035  -3.08162  H
 N-NA--0.279500       0     6.35385  -0.0725   -2.08787  H
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H-H-0.271900          0     8.71286  -4.18318  -1.5647   L
H-H1-0.136000         0     5.88983  -4.41497  -1.64457  L
H-HC-0.036700         0     6.15142  -3.57859  -4.02001  H
H-HC-0.036700         0     7.86586  -3.62054  -3.81452  H
H-H4-0.186200         0     5.40547  -1.74058  -1.16123  H
H-H-0.333900          0     5.76236   0.6945   -1.75769  H
H-H5-0.143500         0     7.64627   0.97477  -3.4479   H
N-N--0.415700         0     7.37163  -6.58178  -3.6724   L
C-CT-0.033700         -1    7.16628  -7.81544  -4.42756  L
C-C-0.597300          0     6.35317  -8.8886   -3.69835  L
O-O--0.567900         0     5.51574  -9.53567  -4.32616  L
C-CT--0.182500        0     8.47585  -8.34977  -5.01206  L
H-H-0.271900          0     8.30355  -6.18546  -3.61909  L
H-H1-0.082300         0     6.55436  -7.53512  -5.28307  L
H-HC-0.060300         0     9.02958  -7.5398   -5.48814  L
H-HC-0.060300         0     8.24787  -9.10497  -5.76553  L
H-HC-0.060300         0     9.07607  -8.81782  -4.23731  L
N-N--0.347900         0     6.52545  -9.05686  -2.38247  L
C-CT--0.240000        -1    5.63065  -9.91621  -1.59682  L
C-C-0.734100          0     4.15996  -9.44521  -1.64391  L
O-O--0.589400         0     3.27578  -10.27943  -1.81756  L
C-CT--0.009400        0     6.1494   -10.08147  -0.15829  L
C-CT-0.018700         0     5.25996  -11.0374   0.66294  L
C-CT--0.047900        0     5.88713  -11.3644   2.02243  L
C-CT--0.014300        0     4.91917  -12.14464   2.92022  L
N-N3--0.385400        0     5.50318  -12.37777   4.26619  L
H-H-0.274700          0     7.21552  -8.46683  -1.92276  L
H-H1-0.142600         0     5.63253  -10.90286  -2.06371  L
H-HC-0.036200         0     6.18434  -9.10884   0.33277  L
H-HC-0.036200         0     7.16299  -10.48389  -0.20139  L
H-HC-0.010300         0     5.11141  -11.96598   0.10939  L
H-HC-0.010300         0     4.28966  -10.56813   0.82933  L
H-HC-0.062100         0     6.14221  -10.426    2.51314  L
H-HC-0.062100         0     6.7928   -11.9518   1.86425  L
H-HP-0.113500         0     4.65394  -13.09139   2.44095  L
H-HP-0.113500         0     4.00572  -11.54915   3.0263   L
H-H-0.340000          0     4.78259  -12.64252   4.93381  L
H-H-0.340000          0     5.86887  -11.49745   4.62946  L
H-H-0.340000          0     6.24671  -13.05781   4.25405  L
N-N--0.415700         0     3.88595  -8.14378  -1.48819  L
C-CT--0.024900        -1    2.53897  -7.55402  -1.65533  L
C-C-0.597300          0     1.98198  -7.79475  -3.0692   L
O-O--0.567900         0     0.85018  -8.26022  -3.17476  L
C-CT-0.211700         0     2.52574  -6.05847  -1.30534  L
O-OH--0.654600        0     1.18313  -5.62225  -1.21675  L
H-H-0.271900          0     4.67991  -7.51953  -1.43263  L
H-H1-0.084300         0     1.8663   -8.0559   -0.95886  L
H-H1-0.035200         0     3.05201  -5.48323  -2.06613  L
H-H1-0.035200         0     3.01437  -5.91322  -0.34281  L
H-HO-0.427500         0     1.1278   -4.70418  -0.88372  L
N-N--0.415700         0     2.75853  -7.55848  -4.14436  L
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C-CT--0.059700       -1    2.41828  -7.9587   -5.53657  L
C-C-0.597300         0     1.98682  -9.44359  -5.53324  L
O-O--0.567900        0     0.85576  -9.74388  -5.89442  L
C-CT-0.130300        0     3.56885  -7.68264  -6.53609  L
C-CT--0.043000       0     3.97564  -6.19343  -6.52335  L
C-CT--0.320400       0     3.15546  -8.09507  -7.96151  L
C-CT--0.066000       0     5.20774  -5.86627  -7.3733   L
H-H-0.271900         0     3.66661  -7.14309  -3.96322  L
H-H1-0.086900        0     1.55293  -7.37496  -5.85265  L
H-HC-0.018700        0     4.43312  -8.27898  -6.25007  L
H-HC-0.023600        0     4.20331  -5.88825  -5.50497  L
H-HC-0.023600        0     3.14083  -5.58981  -6.8763   L
H-HC-0.088200        0     2.3335   -7.46997  -8.31227  L
H-HC-0.088200        0     2.84596  -9.13988  -7.99459  L
H-HC-0.088200        0     3.99563  -7.985    -8.64653  L
H-HC-0.018600        0     4.94814  -5.8645   -8.43201  L
H-HC-0.018600        0     6.00088  -6.59086  -7.19563  L
H-HC-0.018600        0     5.56731  -4.87798  -7.09606  L
N-N--0.415700        0     2.8417   -10.37038  -5.08046  L
C-CT-0.021300        -1    2.60405  -11.82647  -5.11126  L
C-C-0.597300         0     1.37774  -12.32939  -4.35089  L
O-O--0.567900        0     0.8126   -13.35153  -4.72496  L
C-CT--0.123100       -1    3.90675  -12.58471  -4.71341  L
S-SH--0.311900       0     5.2524   -12.2369  -5.88272  L
H-H-0.271900         0     3.75085  -10.04777  -4.77276  L
H-H1-0.112400        0     2.401    -12.08934  -6.1514   L
H-H1-0.111200        0     3.70166  -13.65719  -4.72753  L
H-H1-0.111200        0     4.20472  -12.29672  -3.70449  L
H-HS-0.193300        0     5.42748  -10.95158  -5.54149  L
N-N--0.415700        0     0.96256  -11.63777  -3.29402  L
C-CT--0.051800       -1   -0.27353  -11.94454  -2.58015  L
C-C-0.597300         0    -1.49796  -11.27727  -3.23333  L
O-O--0.567900        0    -2.48243  -11.96657  -3.47473  L
C-CT--0.110200       0    -0.12008  -11.49525  -1.1158   L
C-CT-0.353100        0     0.89227  -12.34285  -0.32062  L
C-CT--0.412100       0     1.24618  -11.63736   0.98652  L
C-CT--0.412100       0     0.3397   -13.7271   0.02639  L
H-H-0.271900         0     1.51628  -10.83624  -3.01819  L
H-H1-0.092200        0    -0.45674  -13.01957  -2.60471  L
H-HC-0.045700        0    -1.09094  -11.55392  -0.62147  L
H-HC-0.045700        0     0.19563  -10.45022  -1.10514  L
H-HC--0.036100       0     1.81186  -12.46724  -0.89156  L
H-HC-0.100000        0     1.70106  -10.67651   0.75027  L
H-HC-0.100000        0     1.95092  -12.23895   1.55571  L
H-HC-0.100000        0     0.3435   -11.46902   1.57574  L
H-HC-0.100000        0     1.06903  -14.28372   0.61253  L
H-HC-0.100000        0     0.13723  -14.28593  -0.88699  L
H-HC-0.100000        0    -0.58583  -13.63006   0.59484  L
N-N--0.415700        0    -1.45826  -9.97081  -3.54009  L
C-CT-0.014300        -1   -2.55446  -9.25612  -4.224    L
C-C-0.597300         0    -2.92332  -9.9168   -5.53796  L
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O-O--0.567900        0    -4.07723  -10.29392  -5.74419  L
C-CT--0.204100       0    -2.27455  -7.75336  -4.30538  L
C-C-0.713000         0    -2.47629  -7.09264  -2.94955  L
O-O--0.593100        0    -3.58207  -6.77856  -2.53319  L
N-N--0.919100        0    -1.42448  -6.86107  -2.20481  L
H-H-0.271900         0    -0.59749  -9.46884  -3.35615  L
H-H1-0.104800        0    -3.44712  -9.37377  -3.60433  L
H-HC-0.079700        0    -2.99055  -7.30808  -4.99415  L
H-HC-0.079700        0    -1.27149  -7.56364  -4.68479  L
H-H-0.419600         0    -1.5507   -6.37387  -1.3382   L
H-H-0.419600         0    -0.50615  -7.14069  -2.52294  L
N-N--0.415700        0    -1.91512  -10.14521  -6.36777  L
C-CT--0.002400       -1   -2.06758  -10.94795  -7.55997  L
C-C-0.597300         0    -2.27168  -12.44397  -7.33687  L
O-O--0.567900        0    -2.76436  -13.1333  -8.22417  L
C-CT--0.034300       0    -0.93088  -10.65923  -8.55614  L
C-CA-0.011800        0    -1.05135  -9.29764  -9.22431  L
C-CA--0.125600       0    -1.78505  -9.17047  -10.41976  L
C-CA--0.125600       0    -0.48943  -8.14817  -8.6351   L
C-CA--0.170400       0    -1.97026  -7.9066   -11.00887  L
C-CA--0.170400       0    -0.66501  -6.88512  -9.23049  L
C-CA--0.107200       0    -1.41393  -6.76259  -10.41292  L
H-H-0.271900         0    -0.98659  -9.8252   -6.11844  L
H-H1-0.097800        0    -2.98561  -10.62202  -8.05233  L
H-HC-0.029500        0    -0.95743  -11.41608  -9.34155  L
H-HC-0.029500        0     0.03563  -10.75245  -8.06361  L
H-HA-0.133000        0    -2.23827  -10.0403  -10.87366  L
H-HA-0.133000        0     0.05574  -8.22917  -7.71033  L
H-HA-0.143000        0    -2.56659  -7.80724  -11.9065  L
H-HA-0.143000        0    -0.2482   -6.00169  -8.77333  L
H-HA-0.129700        0    -1.57967  -5.79014  -10.857   L
N-N--0.415700        0    -1.93711  -12.93768  -6.15097  L
C-CT--0.025200       -1   -2.16099  -14.3135  -5.74055  L
C-C-0.597300         0    -3.62469  -14.71593  -5.59755  L
O-O--0.567900        0    -3.99042  -15.84275  -5.91831  L
H-H-0.271900         0    -1.56041  -12.30309  -5.46568  L
H-H1-0.069800        0    -1.67202  -14.4806  -4.78169  L
H-H1-0.069800        0    -1.70146  -14.97863  -6.47212  L
N-N--0.415700        0    -4.44969  -13.80501  -5.08354  L
C-CT--0.059700       -1   -5.9111   -13.94917  -5.01811  L
C-C-0.597300         0    -6.57766  -13.88283  -6.39563  L
O-O--0.567900        0    -7.5992   -14.53357  -6.60895  L
C-CT-0.130300        0    -6.45627  -12.91198  -3.98123  L
C-CT--0.043000       0    -6.12952  -13.42282  -2.53737  L
C-CT--0.320400       -1   -7.96911  -12.57241  -4.1251   L
C-CT--0.066000       -1   -5.43675  -12.43382  -1.57026  L
H-H-0.271900         0    -4.02885  -12.93324  -4.78512  L
H-H1-0.086900        0    -6.14369  -14.9473  -4.64477  L
H-HC-0.018700        0    -5.91441  -11.97847  -4.14212  L
H-HC-0.023600        0    -5.47585  -14.29387  -2.59746  L
H-HC-0.023600        0    -7.05108  -13.7689  -2.06755  L
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H-HC-0.088200        0    -8.15332  -12.0815  -5.08285  L
H-HC-0.088200        0    -8.27409  -11.89462  -3.32788  L
H-HC-0.088200        0    -8.56354  -13.4854  -4.07515  L
H-HC-0.018600        0    -4.48207  -12.11578  -1.97979  L
H-HC-0.018600        0    -5.27163  -12.91698  -0.60715  L
H-HC-0.018600        0    -6.07346  -11.56022  -1.43051  L
N-N--0.415700        0    -5.97877  -13.14399  -7.33284  L
C-CT--0.149000       -1   -6.38485  -13.11644  -8.7262   L
H-H-0.271900         0    -5.1344   -12.6637  -7.06439  L
H-H1-0.097600        0    -6.67146  -14.11875  -9.04997  L
H-H1-0.097600        0    -5.55903  -12.7622  -9.34434  L
H-H1-0.097600        0    -7.24069  -12.44758  -8.84174  L
C-CT--0.366200       -1   -8.79655  -9.92943  -10.8398  L
C-C-0.597200         0    -8.03643  -9.26408  -9.75827  L
O-O--0.567900        0    -8.38399  -9.29606  -8.58546  L
H-HC-0.112300        0    -8.16496  -10.64925  -11.35491  L
H-HC-0.112300        0    -9.17925  -9.17635  -11.52693  L
H-HC-0.112300        0    -9.64355  -10.44618  -10.38681  L
N-N--0.415700        0    -6.97181  -8.64521  -10.2119  L
C-CT-0.021300        -1   -6.16985  -7.79092  -9.39416  L
C-C-0.597300         0    -5.66683  -6.62716  -10.24697  L
O-O--0.567900        0    -5.06527  -6.87023  -11.29684  L
C-CT--0.123100       0    -4.97427  -8.59486  -8.86026  L
S-SH--0.311900       0    -3.88224  -7.52371  -7.86826  L
H-H-0.271900         0    -6.79113  -8.65068  -11.2028  L
H-H1-0.112400        0    -6.75295  -7.40945  -8.55704  L
H-H1-0.111200        0    -4.41294  -9.00627  -9.6986   L
H-H1-0.111200        0    -5.34146  -9.42179  -8.25211  L
H-HS-0.193300        0    -3.39532  -6.80986  -8.89647  L
N-N--0.415700        0    -5.87458  -5.38549  -9.80578  L
C-CT-0.014300        -1   -5.40707  -4.21382  -10.54194  L
C-C-0.597300         0    -4.03722  -3.67261  -10.04602  L
O-O--0.567900        0    -3.4476   -4.15687  -9.07512  L
C-CT--0.204100       0    -6.53291  -3.16469  -10.64006  L
C-C-0.713000         0    -6.33863  -2.17781  -11.79015  L
O-O--0.593100        0    -5.49977  -2.35893  -12.66302  L
N-N--0.919100        0    -7.05023  -1.08589  -11.82187  L
H-H-0.271900         0    -6.40126  -5.26087  -8.946    L
H-H1-0.104800        0    -5.22249  -4.53502  -11.56874  L
H-HC-0.079700        0    -6.62862  -2.61898  -9.70179  L
H-HC-0.079700        0    -7.46734  -3.68678  -10.8343  L
H-H-0.419600         0    -6.92736  -0.47327  -12.59852  L
H-H-0.419600         0    -7.83678  -0.95699  -11.16973  L
N-N--0.415700        0    -3.49927  -2.6574   -10.72203  L
C-CT--0.051800       -1   -2.32375  -1.87638  -10.34079  L
C-C-0.597300         0    -2.77918  -0.41634  -10.05826  L
O-O--0.567900        0    -3.17486   0.2827   -10.98838  L
C-CT--0.110200       0    -1.27749  -1.95251  -11.47153  L
C-CT-0.353100        0    -0.07524  -1.00134  -11.29664  L
C-CT--0.412100       0     0.7434   -1.32594  -10.04725  L
C-CT--0.412100       0     0.85837  -1.10575  -12.50309  L
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H-H-0.271900          0    -4.02836  -2.32928  -11.52683  L
H-H1-0.092200         0    -1.88691  -2.28072  -9.42722  L
H-HC-0.045700         0    -1.7726   -1.69869  -12.41087  L
H-HC-0.045700         0    -0.91838  -2.97951  -11.54857  L
H-HC--0.036100        0    -0.42013   0.02964  -11.23051  L
H-HC-0.100000         0     1.08029  -2.36145  -10.08724  L
H-HC-0.100000         0     0.13619  -1.17151  -9.15598  L
H-HC-0.100000         0     1.60437  -0.66095  -9.98955  L
H-HC-0.100000         0     1.25049  -2.11929  -12.58833  L
H-HC-0.100000         0     1.68084  -0.40115  -12.38848  L
H-HC-0.100000         0     0.30534  -0.85585  -13.40887  L
N-N--0.347900         0    -2.72983   0.06083  -8.79999  L
C-CT--0.263700        -1   -3.43841   1.28169  -8.32792  L
C-C-0.734100          0    -2.49849   2.31487  -7.73374  L
O-O--0.589400         0    -2.02514   2.14164  -6.62261  L
C-CT--0.000700        0    -4.5023    0.84592  -7.31019  L
C-CT-0.039000         0    -5.51293   1.95375  -6.9797   L
C-CT-0.048600         0    -6.23245   1.64638  -5.66353  L
N-N2--0.529500        0    -5.408     2.01549  -4.49649  L
C-CA-0.807600         0    -5.79708   2.01631  -3.24027  L
N-N2--0.862700        0    -6.94959   1.58738  -2.85151  L
N-N2--0.862700        0    -5.02794   2.44855  -2.29983  L
H-H-0.274700          0    -2.30043  -0.52972  -8.09439  L
H-H1-0.156000         0    -3.95828   1.74246  -9.17029  L
H-HC-0.032700         0    -3.99331   0.52677  -6.40009  L
H-HC-0.032700         0    -5.05755  -0.00584  -7.7075   L
H-HC-0.028500         0    -6.24649   2.01114  -7.78539  L
H-HC-0.028500         0    -5.01722   2.92208  -6.8935   L
H-H1-0.068700         0    -6.52133   0.59711  -5.62798  L
H-H1-0.068700         0    -7.1578    2.20693  -5.63462  L
H-H-0.345600          0    -4.52055   2.50627  -4.63204  L
H-H-0.447800          0    -7.19824   1.64768  -1.87408  L
H-H-0.447800          0    -7.45685   0.91329  -3.42329  L
H-H-0.447800          0    -5.3124    2.32167  -1.34256  L
H-H-0.447800          0    -4.10958   2.82989  -2.54719  L
N-N--0.415700         0    -2.20767   3.3774   -8.47007  L
C-CT--0.002400        -1   -1.30506   4.41685  -7.98393  L
C-C-0.597300          0    -1.88657   5.19379  -6.79114  L
O-O--0.567900         0    -3.00266   5.69741  -6.8653   L
C-CT--0.034300        0    -0.89135   5.3318   -9.14153  L
C-CA-0.011800         0     0.04328   4.62967  -10.11164  L
C-CA--0.125600        0     1.43304   4.65033  -9.88453  L
C-CA--0.125600        0    -0.47271   3.89836  -11.19913  L
C-CA--0.170400        0     2.30094   3.95444  -10.74569  L
C-CA--0.170400        0     0.39359   3.18952  -12.05064  L
C-CA--0.107200        0     1.78107   3.21854  -11.82561  L
H-H-0.271900          0    -2.66583   3.49048  -9.35755  L
H-H1-0.097800         0    -0.39676   3.93562  -7.62318  L
H-HC-0.029500         0    -0.37842   6.20446  -8.73366  L
H-HC-0.029500         0    -1.77939   5.68835  -9.66637  L
H-HA-0.133000         0     1.82917   5.19808  -9.04102  L
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 H-HA-0.133000        0    -1.5388    3.86805  -11.37609  L
 H-HA-0.143000        0     3.3649    3.9857   -10.57271  L
 H-HA-0.143000        0    -0.01603   2.62336  -12.87579  L
 H-HA-0.129700        0     2.44204   2.67681  -12.48536  L
 N-N--0.516300        0    -1.10456   5.30335  -5.71122  L
 C-CT-0.038100        0    -1.46657   6.01857  -4.48187  L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.61855   7.29888  -4.35716  L
 O-O--0.581900        0     0.31728   7.38016  -3.54995  L
 C-CT--0.030300       0    -1.32433   5.08997  -3.26415  H
 C-C-0.799400         0    -2.38635   4.00756  -3.14904  H
 O-O2--0.801400       0    -2.44951   3.40861  -1.95457  H
 O-O2--0.801400       0    -3.17766   3.65386  -3.99018  H
 H-H-0.293600         0    -0.21407   4.82111  -5.72834  L
 H-H1-0.088000        0    -2.51226   6.32985  -4.53492  L
 H-HC--0.012200       0    -1.39684   5.69221  -2.35035  H
 H-HC--0.012200       0    -0.33503   4.61524  -3.26357  H
 N-N--0.516300        0    -0.95588   8.28795  -5.1895   L
 C-CT-0.038100        0    -0.2172    9.52642  -5.49315  L
 C-C-0.536600         0    -0.68048   10.75708  -4.68885  L
 O-O--0.581900        0    -0.33325   11.89522  -5.00398  L
 C-CT--0.030300       0    -0.34148   9.79986  -7.00526  L
 C-C-0.799400         0    -1.72452   10.30181  -7.44026  L
 O-O2--0.801400       0    -2.72093   9.84319  -6.83545  L
 O-O2--0.801400       0    -1.76533   11.09167  -8.40953  L
 H-H-0.293600         0    -1.79061   8.1793   -5.76486  L
 H-H1-0.088000        0     0.83381   9.37096  -5.26439  L
 H-HC--0.012200       0    -0.13274   8.88174  -7.5524   L
 H-HC--0.012200       0     0.41274   10.53688  -7.28787  L
 N-N--0.415700        0    -1.42182   10.5219  -3.6046   L
 C-CT--0.038900       -1   -2.14347   11.48343  -2.74527  L
 C-C-0.597300         0    -1.2461    12.64265  -2.18559  L
 O-O--0.567900        0    -1.78748   13.61383  -1.66125  L
 C-CT-0.365400        0    -2.82036   10.74108  -1.60005  L
 O-OH--0.676100       0    -1.96516   9.80769  -0.96515  L
 C-CT--0.243800       -1   -3.95368   9.95679  -2.23528  L
 H-H-0.271900         0    -1.60454   9.54581  -3.42728  L
 H-H1-0.100700        0    -2.91222   11.97053  -3.34484  L
 H-H1-0.004300        0    -3.21908   11.44035  -0.8658   L
 H-HC-0.064200        0    -4.64227   10.63697  -2.73533  L
 H-HC-0.064200        0    -4.47803   9.43696  -1.44014  L
 H-HC-0.064200        0    -3.58386   9.21887  -2.94702  L
 H-HO-0.410200        0    -1.52747   10.27369  -0.21152  L
 N-N--0.415700        0     0.09978   12.6265  -2.34042  L
 C-CT-0.014300        -1    1.02849   13.78411  -2.19441  L
 C-C-0.597300         0     1.97198   13.89603  -3.41881  L
 O-O--0.567900        0     3.10672   13.41717  -3.33593  L
 C-CT--0.204100       0     1.72061   13.77202  -0.81716  L
 C-C-0.713000         0     2.82544   14.8167  -0.71501  L
 O-O--0.593100        0     2.8729    15.81026  -1.42382  L
 N-N--0.919100        0     3.79203   14.61182   0.14657  L
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H-H-0.271900         0     0.39493   11.86316  -2.93652  L
H-H1-0.104800        0     0.42065   14.68791  -2.1875   L
H-HC-0.079700        0     2.12514   12.78714  -0.61123  L
H-HC-0.079700        0     0.97205   13.98281  -0.05246  L
H-H-0.419600         0     4.47198   15.35009   0.17494  L
H-H-0.419600         0     3.7421    13.87539   0.83811  L
N-N--0.254800        0     1.57384   14.5747  -4.5192   L
C-CT--0.026600      -1     2.32403   14.60178  -5.78624  L
C-C-0.589600         0     3.70308   15.23976  -5.70486  L
O-O--0.574800        0     4.55088   15.00703  -6.56312  L
C-CT--0.007000       0     1.40535   15.26992  -6.81433  L
C-CT-0.018900        0     0.43295   16.08256  -5.96415  L
C-CT-0.019200        0     0.2923    15.24628  -4.69489  L
H-H1-0.064100        0     2.47304   13.56928  -6.10374  L
H-HC-0.025300        0     0.85217   14.49846  -7.35362  L
H-HC-0.025300        0     1.95301   15.90014  -7.51636  L
H-HC-0.021300        0    -0.52615   16.21929  -6.46484  L
H-HC-0.021300        0     0.88019   17.04662  -5.71774  L
H-H1-0.039100        0     0.05384   15.89797  -3.85441  L
H-H1-0.039100        0    -0.49396   14.50117  -4.82895  L
N-N--0.415700        0     3.98555   16.01959  -4.66402  L
C-CT--0.025200      -1     5.19033   16.8349   -4.60612  L
C-C-0.597300         0     6.48084   16.14354  -4.17136  L
O-O--0.567900        0     7.34309   16.7381   -3.53028  L
H-H-0.271900         0     3.298     16.09672  -3.92505  L
H-H1-0.069800        0     5.01208   17.65192  -3.90699  L
H-H1-0.069800        0     5.36874   17.28138  -5.58508  L
N-N--0.347900        0     6.6099    14.88738  -4.57236  L
C-CT--0.240000      -1     7.7582    13.98256  -4.46612  L
C-C-0.734100         0     7.65783   12.91329  -5.5876   L
O-O--0.589400        0     8.40786   11.93748  -5.55768  L
C-CT--0.009400       0     7.74015   13.35467  -3.03956  L
C-CT-0.018700        0     6.48759   12.4846   -2.82126  L
C-CT--0.047900       0     6.25782   11.78141  -1.47852  L
C-CT--0.014300       0     5.20626   10.66671  -1.68911  L
N-N3--0.385400       0     3.83226   11.169    -1.92365  L
H-H-0.274700         0     5.79148   14.56904  -5.07891  L
H-H1-0.142600        0     8.68406   14.54113  -4.60638  L
H-HC-0.036200        0     7.76051   14.14968  -2.29216  L
H-HC-0.036200        0     8.63022   12.73825  -2.90617  L
H-HC-0.010300        0     6.56558   11.6902   -3.5435   L
H-HC-0.010300        0     5.6037    13.07982  -3.0338   L
H-HC-0.062100        0     5.92825   12.49437  -0.7208   L
H-HC-0.062100        0     7.19163   11.32044  -1.15279  L
H-HP-0.113500        0     5.19782   9.99758   -0.82979  L
H-HP-0.113500        0     5.50954   10.07351  -2.55752  L
H-H-0.340000         0     3.30979   10.54994  -2.55584  L
H-H-0.340000         0     3.83218   12.02693  -2.47449  L
H-H-0.340000         0     3.30445   11.32541  -1.08092  L
N-N--0.516300        0     6.70041   13.03474  -6.52513  L
C-CT-0.039700       -1     6.17168   11.94914  -7.37682  L
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C-C-0.536600          0      6.32312   12.27916  -8.88945  L
O-O--0.581900         0      6.07034   13.40447  -9.30847  L
C-CT-0.056000         0      4.74837   11.50117  -6.95572  L
C-CT-0.013600         0      4.78307   11.21568  -5.44982  L
C-C-0.805400          0      3.85576   10.16782  -4.83139  L
O-O2--0.818800        0      2.77401   10.52692  -4.32975  L
O-O2--0.818800        0      4.37978   9.07376  -4.52458  L
H-H-0.293600          0      6.1761    13.89966  -6.60464  L
H-H1-0.110500         0      6.80874   11.07889  -7.21898  L
H-HC--0.017300        0      4.49238   10.59492  -7.49637  L
H-HC--0.017300        0      4.01562   12.27504  -7.17948  L
H-HC--0.042500        0      4.66696   12.1615  -4.92472  L
H-HC--0.042500        0      5.78028   10.84418  -5.25246  L
N-N--0.415700         0      6.81778   11.32503  -9.70696  L
C-CT--0.149000        -1     7.19221   11.51262  -11.127   L
H-H-0.271900          0      6.9866    10.42001  -9.29699  L
H-H1-0.097600         0      7.95589   12.28844  -11.20465  L
H-H1-0.097600         0      6.3148    11.83317  -11.69271  L
H-H1-0.097600         0      7.57235   10.58044  -11.54593  L
C-CT--0.366200        0      10.14516   1.90309  -12.15946  L
C-C-0.597200          0      9.04236   1.2701   -11.34671  L
O-O--0.567900         0      9.27854   0.86204  -10.21374  L
H-HC-0.112300         0      10.7321   2.53947  -11.5002  L
H-HC-0.112300         0      9.73626   2.50298  -12.96951  L
H-HC-0.112300         0      10.77849   1.11279  -12.55781  L
N-N--0.415700         0      7.83844   1.20946  -11.92299  L
C-CT--0.059700        -1     6.65181   0.5863   -11.31423  L
C-C-0.597300          0      5.89584  -0.28069  -12.33878  L
O-O--0.567900         0      6.09849  -1.49008  -12.36393  L
C-CT-0.130300         0      5.75617   1.61807  -10.56487  L
C-CT--0.043000        0      6.54908   2.32901  -9.43671  L
C-CT--0.320400        0      4.50767   0.93955  -9.95836  L
C-CT--0.066000        0      5.78023   3.41261  -8.67187  L
H-H-0.271900          0      7.77564   1.54971  -12.86815  L
H-H1-0.086900         0      7.00799  -0.1172   -10.56224  L
H-HC-0.018700         0      5.42319   2.37243  -11.27973  L
H-HC-0.023600         0      7.41474   2.82713  -9.8704   L
H-HC-0.023600         0      6.90948   1.58578  -8.72343  L
H-HC-0.088200         0      3.94497   0.38795  -10.70994  L
H-HC-0.088200         0      3.83001   1.68708  -9.54733  L
H-HC-0.088200         0      4.79716   0.2537   -9.16317  L
H-HC-0.018600         0      4.97141   2.97723  -8.08567  L
H-HC-0.018600         0      5.37832   4.14065  -9.37572  L
H-HC-0.018600         0      6.46286   3.92387  -7.99206  L
N-N--0.415700         0      5.03318   0.31127  -13.17904  L
C-CT--0.149000        -1     4.19098  -0.41226  -14.13766  L
H-H-0.271900          0      4.91408   1.30744  -13.09004  L
H-H1-0.097600         0      3.73238  -1.27583  -13.6503  L
H-H1-0.097600         0      4.80046  -0.76951  -14.96957  L
H-H1-0.097600         0      3.40325   0.23898  -14.51967  L
C-CT--0.366200        -1    -4.94433   17.09058  -2.88443  L
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C-C-0.597200         0    -5.51239   16.30436  -1.71617  L
O-O--0.567900        0    -5.31581   16.7127  -0.57476  L
H-HC-0.112300        0    -5.75626   17.51321  -3.47124  L
H-HC-0.112300        0    -4.33155   16.42912  -3.49536  L
H-HC-0.112300        0    -4.31982   17.89204  -2.49397  L
N-N--0.254800        0    -6.26901   15.22578  -1.97577  L
C-CT--0.026600       -1   -6.94661   14.45848  -0.93686  L
C-C-0.589600         0    -6.07896   13.35398  -0.33675  L
O-O--0.574800        0    -5.52157   12.50395  -1.02807  L
C-CT--0.007000       0    -8.15657   13.85481  -1.65968  L
C-CT-0.018900        0    -7.63817   13.60159  -3.07768  L
C-CT-0.019200        0    -6.66207   14.75775  -3.30082  L
H-H1-0.064100        0    -7.29805   15.12153  -0.14567  L
H-HC-0.025300        0    -8.96138   14.59055  -1.69486  L
H-HC-0.025300        0    -8.5076    12.93799  -1.18665  L
H-HC-0.021300        0    -8.44673   13.61033  -3.80899  L
H-HC-0.021300        0    -7.10179   12.65325  -3.12094  L
H-H1-0.039100        0    -5.79518   14.412   -3.86614  L
H-H1-0.039100        0    -7.16805   15.56007  -3.83876  L
N-N--0.415700        0    -6.03237   13.35779   0.98782  L
C-CT--0.023700       -1   -5.18182   12.50699   1.80698  L
C-C-0.597300         0    -5.38598   10.98223   1.65446  L
O-O--0.567900        0    -6.46519   10.51379   1.28532  L
C-CT-0.034200        0    -5.43454   12.86044   3.28663  L
C-CT-0.001800        0    -4.96865   14.26629   3.69041  L
S-S--0.273700        0    -3.17661   14.48012   3.87617  L
C-CT--0.053600       -1   -2.87905   13.52721   5.3933   L
H-H-0.271900         0    -6.53369   14.09826   1.44678  L
H-H1-0.088000        0    -4.13935   12.72468   1.56435  L
H-HC-0.024100        0    -4.93455   12.13485   3.9282   L
H-HC-0.024100        0    -6.505     12.78035   3.48353  L
H-H1-0.044000        0    -5.4326    14.51666   4.64464  L
H-H1-0.044000        0    -5.32569   14.98713   2.9548   L
H-H1-0.068400        0    -3.10032   12.47309   5.22239  L
H-H1-0.068400        0    -3.5058    13.90668   6.19974  L
H-H1-0.068400        0    -1.83008   13.61887   5.67537  L
N-N--0.415700        0    -4.35101   10.21426   2.02717  L
C-CT--0.001400       -1   -4.21674   8.76776   1.81474  L
C-C-0.597300         0    -5.444     7.87747   2.1116   L
O-O--0.567900        0    -6.04061   7.38727   1.15935  L
C-CT--0.015200       0    -2.8942    8.22934   2.38178  L
C-CA--0.001100       0    -2.80236   6.71309   2.4761   L
C-CA--0.190600       0    -2.96212   5.88461   1.34405  L
C-CA--0.190600       0    -2.6735    6.13019   3.74561  L
C-CA--0.234100       0    -3.04263   4.48215   1.50434  L
C-CA--0.234100       0    -2.77318   4.74174   3.91068  L
C-C-0.322600         0    -2.97424   3.91188   2.79527  L
O-OH--0.557900       0    -3.12406   2.57451   2.97551  L
H-H-0.271900         0    -3.51031   10.69344   2.3196   L
H-H1-0.087600        0    -4.09828   8.66594   0.73564  L
H-HC-0.029500        0    -2.75372   8.65324   3.37322  L
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H-HC-0.029500        0    -2.07808   8.58282   1.7537   L
H-HA-0.169900        0    -3.1079    6.33566   0.36959  L
H-HA-0.169900        0    -2.58061   6.75762   4.61802  L
H-HA-0.165600        0    -3.24379   3.83658   0.66003  L
H-HA-0.165600        0    -2.77118   4.33016   4.90738  L
H-HO-0.399200        0    -3.45374   2.40997   3.87973  L
N-N--0.516300        0    -5.80475   7.5825    3.3652   L
C-CT-0.038100        -1   -6.7787    6.52235   3.72679  L
C-C-0.536600         0    -8.18576   6.76803   3.17954  L
O-O--0.581900        0    -8.86533   5.82046   2.79282  L
C-CT--0.030300       0    -6.79737   6.33001   5.2549   L
C-C-0.799400         0    -5.49841   5.70127   5.78104  L
O-O2--0.801400       0    -5.36629   4.45704   5.67689  L
O-O2--0.801400       0    -4.62386   6.46215   6.26851  L
H-H-0.293600         0    -5.29537   8.04838   4.11104  L
H-H1-0.088000        0    -6.42965   5.58291   3.3024   L
H-HC--0.012200       0    -7.6257    5.67034   5.51625  L
H-HC--0.012200       0    -6.97437   7.29019   5.74282  L
N-N--0.415700        0    -8.6051    8.03339   3.10121  L
C-CT--0.002400       0    -9.79469   8.45367   2.35892  L
C-C-0.597300         0    -9.71101   8.02004   0.88686  L
O-O--0.567900        0    -10.57481   7.29309   0.39678  L
C-CT--0.034300       0    -9.97046   9.97401   2.49453  L
C-CA-0.011800        0    -11.02714   10.54736   1.56862  L
C-CA--0.125600       0    -12.39302   10.40781   1.8782   L
C-CA--0.125600       0    -10.64413   11.16666   0.36308  L
C-CA--0.170400       0    -13.37044   10.88991   0.98859  L
C-CA--0.170400       0    -11.62064   11.64609  -0.52717  L
C-CA--0.107200       0    -12.98443   11.50849  -0.2141   L
H-H-0.271900         0    -7.94048   8.73149   3.40128  L
H-H1-0.097800        0    -10.66975   7.96326   2.78717  L
H-HC-0.029500        0    -9.01939   10.46509   2.28276  L
H-HC-0.029500        0    -10.23673   10.20766   3.52609  L
H-HA-0.133000        0    -12.69281   9.91164   2.79017  L
H-HA-0.133000        0    -9.59686   11.24758   0.10395  L
H-HA-0.143000        0    -14.41841   10.76839   1.22196  L
H-HA-0.143000        0    -11.3181   12.10091  -1.45982  L
H-HA-0.129700        0    -13.73516   11.86462  -0.90504  L
N-N--0.415700        0    -8.6749    8.45694   0.17295  L
C-CT--0.038900       -1   -8.50174   8.16603  -1.25469  L
C-C-0.597300         0    -8.35442   6.68595  -1.55596  L
O-O--0.567900        0    -9.01958   6.15163  -2.4407   L
C-CT-0.365400        0    -7.33656   8.97906  -1.83049  L
O-OH--0.676100       0    -7.56301   10.35089  -1.58219  L
C-CT--0.243800       0    -7.20154   8.82271  -3.34565  L
H-H-0.271900         0    -7.98773   9.05798   0.61701  L
H-H1-0.100700        0    -9.40361   8.49823  -1.76857  L
H-H1-0.004300        0    -6.41884   8.66393  -1.34     L
H-HC-0.064200        0    -8.14732   9.06805  -3.82905  L
H-HC-0.064200        0    -6.92056   7.80024  -3.59693  L
H-HC-0.064200        0    -6.4316    9.4939   -3.72352  L
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H-HO-0.410200        0    -6.70946   10.77436  -1.40391  L
N-N--0.415700        0    -7.50996   6.02013  -0.77899  L
C-CT--0.058100       -1   -7.37868   4.57564  -0.68245  L
C-C-0.597300         0    -8.72996   3.88989  -0.54147  L
O-O--0.567900        0    -9.05071   3.03917  -1.3701   L
C-CT--0.007400       0    -6.42076   4.29161   0.4757   L
C-CC-0.186800        0    -6.35186   2.86004   0.9075   L
N-NB--0.543200       0    -6.51607   1.75817   0.07484  L
C-CW--0.220700       0    -6.21865   2.44068   2.19352  L
C-CR-0.163500        0    -6.51057   0.68612   0.87428  L
N-NA--0.279500       0    -6.3173    1.07157   2.14575  L
H-H-0.271900         0    -7.02625   6.57817  -0.08239  L
H-H1-0.136000        0    -6.93682   4.20372  -1.60573  L
H-HC-0.036700        0    -6.74484   4.86932   1.33526  L
H-HC-0.036700        0    -5.42605   4.62821   0.19179  L
H-H4-0.186200        0    -6.10596   3.06402   3.07262  L
H-H-0.333900         0    -6.31059   0.44044   2.94396  L
H-H5-0.143500        0    -6.66795  -0.33292   0.54243  L
N-N--0.415700        0    -9.52643   4.26307   0.46535  L
C-CT-0.021300        -1   -10.82851   3.64272   0.66224  L
C-C-0.597300         0    -11.74362   3.71601  -0.53781  L
O-O--0.567900        0    -12.36815   2.72594  -0.91508  L
C-CT--0.123100       0    -11.47939   4.01806   2.01079  L
S-SH--0.311900       0    -12.54312   5.48867   1.96247  L
H-H-0.271900         0    -9.21783   4.97369   1.12099  L
H-H1-0.112400        0    -10.61541   2.57599   0.7493   L
H-H1-0.111200        0    -10.70553   4.15603   2.76533  L
H-H1-0.111200        0    -12.09549   3.17689   2.33261  L
H-HS-0.193300        0    -11.62027   6.32366   1.46574  L
N-N--0.415700        0    -11.77407   4.88702  -1.15213  L
C-CT--0.059700       -1   -12.59842   5.1341   -2.30735  L
C-C-0.597300         0    -12.13976   4.42058  -3.58014  L
O-O--0.567900        0    -12.96457   3.81715  -4.26248  L
C-CT-0.130300        0    -12.81312   6.66382  -2.46446  L
C-CT--0.043000       0    -14.14204   7.11272  -1.80648  L
C-CT--0.320400       -1   -12.72201   7.18959  -3.90149  L
C-CT--0.066000       -1   -15.43866   6.73176  -2.55221  L
H-H-0.271900         0    -11.22294   5.63936  -0.75347  L
H-H1-0.086900        0    -13.57208   4.69485  -2.09228  L
H-HC-0.018700        0    -12.01286   7.17195  -1.92249  L
H-HC-0.023600        0    -14.12268   8.19854  -1.70301  L
H-HC-0.023600        0    -14.18684   6.69613  -0.79896  L
H-HC-0.088200        0    -11.7064   7.0685   -4.27983  L
H-HC-0.088200        0    -12.95998   8.25317  -3.92002  L
H-HC-0.088200        0    -13.41464   6.65641  -4.55437  L
H-HC-0.018600        0    -16.29794   7.03908  -1.95593  L
H-HC-0.018600        0    -15.48686   5.65415  -2.7083   L
H-HC-0.018600        0    -15.4854   7.23947  -3.51541  L
N-N--0.415700        0    -10.85197   4.49359  -3.91175  L
C-CT--0.024900       -1   -10.2605   3.80419  -5.06401  L
C-C-0.597300         0    -10.48548   2.28144  -4.92725  L
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O-O--0.567900        0    -10.95533   1.65744  -5.87179  L
C-CT-0.211700        0    -8.79717   4.23877  -5.17113  L
O-OH--0.654600       0    -8.32681   4.10753  -6.49597  L
H-H-0.271900         0    -10.24543   5.01935  -3.29066  L
H-H1-0.084300        0    -10.77916   4.13337  -5.96489  L
H-H1-0.035200        0    -8.18317   3.67041  -4.47244  L
H-H1-0.035200        0    -8.72586   5.29475  -4.90654  L
H-HO-0.427500        0    -7.54379   4.6566   -6.60216  L
N-N--0.516300        0    -10.27425   1.68548  -3.73899  L
C-CT-0.038100        -1   -10.59964   0.26753  -3.4641   L
C-C-0.536600         0    -12.08594  -0.09471  -3.60803  L
O-O--0.581900        0    -12.43025  -1.03324  -4.33224  L
C-CT--0.030300       0    -10.07494  -0.1935   -2.08537  L
C-C-0.799400         0    -8.68864  -0.83048  -2.1686   L
O-O2--0.801400       0    -8.07205  -0.78398  -3.25336  L
O-O2--0.801400       0    -8.18449  -1.35509  -1.15116  L
H-H-0.293600         0    -9.92869   2.25433  -2.97324  L
H-H1-0.088000        0    -10.11519  -0.31875  -4.24139  L
H-HC--0.012200       0    -10.75187  -0.94403  -1.67441  L
H-HC--0.012200       0    -10.06127   0.64292  -1.38693  L
N-N--0.415700        0    -12.96384   0.62401  -2.90437  L
C-CT-0.033700        -1   -14.41871   0.49551  -3.0013   L
C-C-0.597300         0    -14.90916   0.53595  -4.46109  L
O-O--0.567900        0    -15.75586  -0.26246  -4.85821  L
C-CT--0.182500       -1   -15.0165   1.65114  -2.25716  L
H-H-0.271900         0    -12.59937   1.3689   -2.31924  L
H-H1-0.082300        0    -14.73855  -0.44608  -2.55427  L
H-HC-0.060300        0    -14.74002   1.59334  -1.20399  L
H-HC-0.060300        0    -16.10415   1.60676  -2.32826  L
H-HC-0.060300        0    -14.67287   2.60063  -2.66639  L
N-N--0.415700        0    -14.40666   1.50992  -5.22685  L
C-CT--0.025200       -1   -14.77391   1.78713  -6.61053  L
C-C-0.597300         0    -14.29652   0.73329  -7.60589  L
O-O--0.567900        0    -15.04647   0.34309  -8.49586  L
H-H-0.271900         0    -13.72777   2.12884  -4.79491  L
H-H1-0.069800        0    -14.34809   2.74567  -6.90454  L
H-H1-0.069800        0    -15.85915   1.85338  -6.68475  L
N-N--0.516300        0    -13.04678   0.29784  -7.46381  L
C-CT-0.039700        -1   -12.42713  -0.7897   -8.22531  L
C-C-0.536600         0    -13.1727  -2.12849  -8.069    L
O-O--0.581900        0    -13.32141  -2.87189  -9.03588  L
C-CT-0.056000        0    -10.96153  -0.87337  -7.76536  L
C-CT-0.013600        0    -10.09689  -1.96152  -8.41066  L
C-C-0.805400         0    -9.63178  -1.64715  -9.83395  L
O-O2--0.818800       0    -9.6563   -2.56448  -10.68501  L
O-O2--0.818800       0    -9.08243  -0.54598  -10.05291  L
H-H-0.293600         0    -12.47248   0.73065  -6.74588  L
H-H1-0.110500        0    -12.44089  -0.5374   -9.28639  L
H-HC--0.017300       0    -10.96894  -1.0522   -6.69215  L
H-HC--0.017300       0    -10.4821   0.09189  -7.92867  L
H-HC--0.042500       0    -10.6396  -2.90215  -8.38281  L
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H-HC--0.042500       0    -9.1999   -2.08386  -7.80125  L
N-N--0.415700        0    -13.62587  -2.4464   -6.85141  L
C-CT--0.025200       -1   -14.33924  -3.68888  -6.51749  L
C-C-0.597300         0    -13.59982  -4.56759  -5.52422  L
O-O--0.567900        0    -13.95335  -5.74033  -5.37951  L
H-H-0.271900         0    -13.49124  -1.74476  -6.13205  L
H-H1-0.069800        0    -14.51692  -4.27599  -7.41892  L
H-H1-0.069800        0    -15.3055  -3.43091  -6.08588  L
N-N--0.415700        0    -12.58229  -4.02714  -4.83708  L
C-CT--0.059700       -1   -11.85079  -4.75812  -3.80159  L
C-C-0.597300         0    -12.86956  -5.30033  -2.7945   L
O-O--0.567900        0    -13.78726  -4.59489  -2.38118  L
C-CT-0.130300        0    -10.75769  -3.891    -3.12442  L
C-CT--0.043000       0    -9.45563  -3.89732  -3.94187  L
C-CT--0.320400       0    -10.34325  -4.40556  -1.72875  L
C-CT--0.066000       0    -9.51581  -3.23146  -5.31046  L
H-H-0.271900         0    -12.41443  -3.0336   -4.95494  L
H-H1-0.086900        0    -11.37501  -5.60517  -4.27851  L
H-HC-0.018700        0    -11.11956  -2.87096  -3.01114  L
H-HC-0.023600        0    -9.1645   -4.92707  -4.08551  L
H-HC-0.023600        0    -8.67314  -3.40498  -3.36872  L
H-HC-0.088200        0    -9.5658   -3.76259  -1.31245  L
H-HC-0.088200        0    -9.96625  -5.42678  -1.79526  L
H-HC-0.088200        0    -11.1856  -4.36804  -1.04572  L
H-HC-0.018600        0    -8.53045  -3.26958  -5.77237  L
H-HC-0.018600        0    -9.80896  -2.194    -5.19307  L
H-HC-0.018600        0    -10.2238  -3.74629  -5.95552  L
N-N--0.415700        0    -12.70101  -6.56219  -2.39631  L
C-CT--0.025200       -1   -13.56001  -7.21455  -1.40004  L
C-C-0.597300         0    -13.00283  -7.17598   0.0061   L
O-O--0.567900        0    -13.72591  -6.98134   0.98111  L
H-H-0.271900         0    -11.96686  -7.07079  -2.87231  L
H-H1-0.069800        0    -13.70136  -8.25678  -1.68176  L
H-H1-0.069800        0    -14.5421  -6.73918  -1.38976  L
N-N--0.415700        0    -11.69586  -7.38147   0.0926   L
C-CT--0.058100       -1   -10.94006  -7.3985    1.3265   L
C-C-0.597300         0    -9.5553   -6.76784   1.06641  L
O-O--0.567900        0    -8.82247  -7.25274   0.2052   L
C-CT--0.007400       0    -10.80717  -8.8509    1.81692  L
C-CC-0.186800        0    -12.10948  -9.43111   2.32032  L
N-NB--0.543200       0    -12.70385  -9.16057   3.55619  L
C-CW--0.220700       0    -12.9359  -10.2436   1.60055  L
C-CR-0.163500        0    -13.88071  -9.80167   3.54554  L
N-NA--0.279500       0    -14.04602  -10.46476   2.38714  L
H-H-0.271900         0    -11.17844  -7.4916   -0.76776  L
H-H1-0.136000        0    -11.45228  -6.81557   2.09359  L
H-HC-0.036700        0    -10.06923  -8.89635   2.61536  L
H-HC-0.036700        0    -10.43205  -9.47257   1.00248  L
H-H4-0.186200        0    -12.75701  -10.59349   0.59402  L
H-H-0.333900         0    -14.86904  -10.98987   2.13144  L
H-H5-0.143500        0    -14.59895  -9.77524   4.35493  L
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N-N--0.415700        0    -9.19485  -5.67578   1.75293  L
C-CT--0.024900       -1   -7.92842  -4.95061   1.52663  L
C-C-0.597300         0    -6.73895  -5.59958   2.23624  L
O-O--0.567900        0    -6.77441  -5.87538   3.43509  L
C-CT-0.211700        0    -8.04295  -3.46127   1.87332  L
O-OH--0.654600       0    -6.75881  -2.84993   1.8471   L
H-H-0.271900         0    -9.80813  -5.38098   2.50487  L
H-H1-0.084300        0    -7.72103  -4.98625   0.4564   L
H-H1-0.035200        0    -8.48396  -3.35402   2.85753  L
H-H1-0.035200        0    -8.69539  -2.96906   1.1496   L
H-HO-0.427500        0    -6.76817  -2.092     2.46175  L
N-N--0.415700        0    -5.65465  -5.80919   1.48691  L
C-CT--0.051800       -1   -4.35347  -6.22061   2.00998  L
C-C-0.597300         0    -3.46466  -5.01414   2.25309  L
O-O--0.567900        0    -3.25443  -4.21592   1.34231  L
C-CT--0.110200       0    -3.67292  -7.19822   1.02815  L
C-CT-0.353100        0    -4.20184  -8.6458    1.02482  L
C-CT--0.412100       0    -5.57718  -8.79725   0.37402  L
C-CT--0.412100       0    -3.22539  -9.52923   0.2413   L
H-H-0.271900         0    -5.73897  -5.60161   0.50349  L
H-H1-0.092200        0    -4.49226  -6.73578   2.96371  L
H-HC-0.045700        0    -2.62132  -7.24627   1.30133  L
H-HC-0.045700        0    -3.72227  -6.79612   0.01963  L
H-HC--0.036100       0    -4.2484   -9.0132    2.05024  L
H-HC-0.100000        0    -5.57167  -8.37278  -0.63056  L
H-HC-0.100000        0    -6.33552  -8.29603   0.97305  L
H-HC-0.100000        0    -5.84841  -9.85027   0.31682  L
H-HC-0.100000        0    -2.2365   -9.48351   0.69674  L
H-HC-0.100000        0    -3.16562  -9.1895   -0.79326  L
H-HC-0.100000        0    -3.57124  -10.56265   0.25699  L
N-N--0.415700        0    -2.90331  -4.92137   3.45085  L
C-CT-0.021300        -1   -1.95561  -3.8741    3.8014   L
C-C-0.597300         0    -0.82285  -4.41437   4.69243  L
O-O--0.567900        0    -0.83558  -5.58111   5.08765  L
C-CT--0.123100       0    -2.759    -2.74736   4.45969  L
S-SH--0.311900       0    -1.80512  -1.21007   4.53372  L
H-H-0.271900         0    -3.15484  -5.59646   4.16494  L
H-H1-0.112400        0    -1.49196  -3.47799   2.89462  L
H-H1-0.111200        0    -3.068    -3.04517   5.46324  L
H-H1-0.111200        0    -3.65026  -2.55673   3.86087  L
H-HS-0.193300        0    -2.71737  -0.51764   5.23045  L
N-N--0.415700        0     0.16957  -3.59202   5.0309   L
C-CT--0.038900       -1    1.28241  -3.98619   5.90726  L
C-C-0.597300         0     1.40563  -3.12218   7.13855  L
O-O--0.567900        0     0.72905  -2.1165    7.33041  L
C-CT-0.365400        0     2.6326   -4.08169   5.16937  L
O-OH--0.676100       0     3.01489  -2.86841   4.55652  L
C-CT--0.243800       0     2.6292   -5.20256   4.13366  L
H-H-0.271900         0     0.08517  -2.6272    4.7337   L
H-H1-0.100700        0     1.07835  -4.98631   6.28991  L
H-H1-0.004300        0     3.40946  -4.33969   5.88908  L
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H-HC-0.064200        0     1.9046   -4.99996   3.34687  L
H-HC-0.064200        0     2.36546  -6.14599   4.61293  L
H-HC-0.064200        0     3.62059  -5.29151   3.69976  L
H-HO-0.410200        0     3.3782   -2.28017   5.25754  L
N-N--0.415700        0     2.25897  -3.61329   8.02647  L
C-CT--0.051800       -1    2.1798   -3.33124   9.43639  L
C-C-0.597300         0     2.2803   -1.83755   9.83289  L
O-O--0.567900        0     1.72902  -1.454     10.85539  L
C-CT--0.110200       0     3.18104  -4.21726   10.14563  L
C-CT-0.353100        0     2.88346  -4.31387   11.64348  L
C-CT--0.412100       0     1.53896  -4.95795   11.99313  L
C-CT--0.412100       -1    3.97255  -5.22287   12.14928  L
H-H-0.271900         0     2.7216   -4.46445   7.76141  L
H-H1-0.092200        0     1.17658  -3.63564   9.73633  L
H-HC-0.045700        0     4.18036  -3.80834   9.98787  L
H-HC-0.045700        0     3.13432  -5.21987   9.7154   L
H-HC--0.036100       0     2.97939  -3.34451   12.12938  L
H-HC-0.100000        0     1.41235  -5.90523   11.4702  L
H-HC-0.100000        0     0.72189  -4.28845   11.73178  L
H-HC-0.100000        0     1.47778  -5.12555   13.06946  L
H-HC-0.100000        0     3.867    -5.3292    13.2298  L
H-HC-0.100000        0     4.95231  -4.78975   11.95067  L
H-HC-0.100000        0     3.89698  -6.21102   11.69541  L
N-N--0.516300        0     2.9516   -0.98634   9.05173  L
C-CT-0.039700        -1    3.09582   0.46146   9.3217   L
C-C-0.536600         0     1.85743   1.32958   8.99491  L
O-O--0.581900        0     1.95125   2.56009   8.95692  L
C-CT-0.056000        0     4.36221   0.97407   8.59742  L
C-CT-0.013600        0     4.34723   0.90293   7.05678  L
C-C-0.805400         0     4.91445  -0.40671   6.49224  L
O-O2--0.818800       0     4.234    -1.46118   6.50597  L
O-O2--0.818800       0     6.09482  -0.42571   6.05964  L
H-H-0.293600         0     3.28262  -1.34043   8.15837  L
H-H1-0.110500        0     3.25825   0.59275   10.39259  L
H-HC--0.017300       0     5.22999   0.42439   8.96626  L
H-HC--0.017300       0     4.51263   2.01569   8.8834   L
H-HC--0.042500       0     4.96902   1.71815   6.68386  L
H-HC--0.042500       0     3.33807   1.06712   6.68687  L
N-N--0.415700        0     0.70206   0.69333   8.78997  L
C-CT--0.002400       -1   -0.60843   1.31982   8.58068  L
C-C-0.597300         0    -1.74809   0.67529   9.38503  L
O-O--0.567900        0    -2.92285   0.99612   9.19782  L
C-CT--0.034300       0    -0.97643   1.17322   7.08987  L
C-CA-0.011800        0    -0.01843   1.68643   6.02474  L
C-CA--0.125600       0    -0.18874   2.97784   5.49765  L
C-CA--0.125600       0     0.93895   0.83038   5.44524  L
C-CA--0.170400       0     0.57025   3.39907   4.39243  L
C-CA--0.170400       0     1.73309   1.26688   4.36815  L
C-CA--0.107200       0     1.55126   2.55631   3.84079  L
H-H-0.271900         0     0.74978  -0.31548   8.73249  L
H-H1-0.097800        0    -0.56217   2.37781   8.83793  L
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H-HC-0.029500        0    -1.93335   1.66828   6.92628  L
H-HC-0.029500        0    -1.1418    0.11237   6.90453  L
H-HA-0.133000        0    -0.92957   3.6381    5.92364  L
H-HA-0.133000        0     1.0537   -0.17445   5.81903  L
H-HA-0.143000        0     0.38622   4.37926   3.98113  L
H-HA-0.143000        0     2.46591   0.60152   3.93519  L
H-HA-0.129700        0     2.15857   2.89092   3.01111  L
N-N--0.415700        0    -1.39118  -0.24755   10.26746  L
C-CT--0.003100      -1    -2.25845  -1.13068   11.02923  L
C-C-0.597300         0    -3.49818  -0.43448   11.64956  L
O-O--0.567900        0    -4.64087  -0.76207   11.34695  L
C-CT--0.003600       0    -1.33898  -1.73897   12.10884  L
C-CT--0.064500       0    -1.99595  -2.496     13.27575  L
C-C-0.695100         0    -1.05918  -2.55838   14.48106  L
O-O--0.608600        0    -0.60074  -3.61285   14.88995  L
N-N--0.940700        0    -0.73439  -1.44496   15.10793  L
H-H-0.271900         0    -0.39513  -0.33858   10.42265  L
H-H1-0.085000        0    -2.63589  -1.92163   10.3942  L
H-HC-0.017100        0    -0.75306  -0.92154   12.53285  L
H-HC-0.017100        0    -0.63577  -2.41264   11.62121  L
H-HC-0.035200        0    -2.24857  -3.50619   12.95248  L
H-HC-0.035200        0    -2.91034  -2.00744   13.60473  L
H-H-0.425100         0    -0.10111  -1.57741   15.86998  L
H-H-0.425100         0    -1.00208  -0.50741   14.79692  L
N-N--0.516300        0    -3.27346   0.47027   12.59616  L
C-CT-0.038100       -1    -4.23398   1.3419    13.30949  L
C-C-0.536600         0    -4.79968   2.43396   12.39884  L
O-O--0.581900        0    -5.98678   2.74978   12.47117  L
C-CT--0.030300       0    -3.49207   1.95825   14.51424  L
C-C-0.799400         0    -2.02765   2.25198   14.16656  L
O-O2--0.801400       0    -1.76857   3.26066   13.47301  L
O-O2--0.801400       0    -1.19639   1.33124   14.36843  L
H-H-0.293600         0    -2.29318   0.6084    12.81806  L
H-H1-0.088000        0    -5.07476   0.75041   13.67293  L
H-HC--0.012200       0    -3.51874   1.24401   15.33923  L
H-HC--0.012200       0    -3.99525   2.86998   14.84063  L
N-N--0.415700        0    -3.95285   2.98389   11.52351  L
C-CT-0.014300       -1    -4.30261   4.01672   10.55211  L
C-C-0.597300         0    -5.55979   3.69791   9.74362  L
O-O--0.567900        0    -6.34407   4.59266   9.42797  L
C-CT--0.204100       0    -3.1098    4.32679   9.62575  L
C-C-0.713000         0    -2.07723   5.2906    10.18286  L
O-O--0.593100        0    -1.6274    6.1875    9.48868  L
N-N--0.919100        0    -1.61449   5.15179   11.40389  L
H-H-0.271900         0    -2.9961    2.66706   11.58225  L
H-H1-0.104800        0    -4.54258   4.92844   11.10248  L
H-HC-0.079700        0    -3.50086   4.78835   8.71648  L
H-HC-0.079700        0    -2.6059    3.41717   9.32745  L
H-H-0.419600         0    -0.94478   5.85175   11.65448  L
H-H-0.419600         0    -1.89786   4.43907   12.07964  L
N-N--0.347900        0    -5.7631    2.41529   9.43708  L
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C-CT--0.263700       -1   -6.91248   1.9329    8.68027  L
C-C-0.734100         0    -8.30485   2.24909   9.2439   L
O-O--0.589400        0    -9.29421   2.07012   8.53667  L
C-CT--0.000700       0    -6.74697   0.43439   8.36978  L
C-CT-0.039000        0    -7.34305  -0.46439   9.45751  L
C-CT-0.048600        0    -6.95     -1.9263    9.26407  L
N-N2--0.529500       0    -7.62491  -2.73875   10.28222  L
C-CA-0.807600        0    -7.11241  -3.14207   11.41905  L
N-N2--0.862700       0    -5.83961  -3.24884   11.63499  L
N-N2--0.862700       0    -7.89584  -3.39277   12.41854  L
H-H-0.274700         0    -5.03662   1.76467   9.7163   L
H-H1-0.156000        0    -6.87891   2.45512   7.7221   L
H-HC-0.032700        0    -5.68657   0.2052    8.24869  L
H-HC-0.032700        0    -7.25381   0.21333   7.42888  L
H-HC-0.028500        0    -8.43134  -0.39447   9.43089  L
H-HC-0.028500        0    -6.99734  -0.12871   10.4356  L
H-H1-0.068700        0    -5.86833  -2.00437   9.34632  L
H-H1-0.068700        0    -7.24634  -2.26711   8.27543  L
H-H-0.345600         0    -8.63461  -2.79197   10.23593  L
H-H-0.447800         0    -5.462    -2.31495   11.74845  L
H-H-0.447800         0    -5.36846  -3.59052   10.78765  L
H-H-0.447800         0    -7.4665   -3.65321   13.28088  L
H-H-0.447800         0    -8.86866  -3.10236   12.32785  L
N-N--0.415700        0    -8.41652   2.69098   10.4932  L
C-CT--0.149000       -1   -9.69688   3.03795   11.08407  L
H-H-0.271900         0    -7.56127   2.80388   11.02646  L
H-H1-0.097600        0    -10.27294   3.66331   10.40094  L
H-H1-0.097600        0    -9.53503   3.57857   12.01724  L
H-H1-0.097600        0    -10.25725   2.12427   11.29277  L
C-CT--0.366200       -1   -9.88253   6.27991   8.93433  L
C-C-0.597200         0    -10.60785   5.56122   7.82074  L
O-O--0.567900        0    -11.78617   5.82432   7.62129  L
H-HC-0.112300        0    -9.06972   5.66175   9.31613  L
H-HC-0.112300        0    -10.58611   6.49777   9.7349   L
H-HC-0.112300        0    -9.47617   7.20981   8.54117  L
N-N--0.415700        0    -9.92792   4.647     7.12531  L
C-CT--0.001400       -1   -10.46284   3.82238   6.0217   L
C-C-0.597300         0    -11.80077   3.13006   6.31979  L
O-O--0.567900        0    -12.67903   3.01143   5.46272  L
C-CT--0.015200       0    -9.33514   2.92445   5.45959  L
C-CA--0.001100       0    -9.73621   1.70104   4.65512  L
C-CA--0.190600       0    -10.36022   0.61552   5.2996   L
C-CA--0.190600       0    -9.41917   1.61208   3.2845   L
C-CA--0.234100       0    -10.72155  -0.52673   4.56627  L
C-CA--0.234100       0    -9.73836   0.44952   2.55505  L
C-C-0.322600         0    -10.40063  -0.61539   3.19703  L
O-OH--0.557900       0    -10.74296  -1.73044   2.50948  L
H-H-0.271900         0    -8.96286   4.50488   7.38282  L
H-H1-0.087600        0    -10.70748   4.51578   5.21534  L
H-HC-0.029500        0    -8.69974   2.5748    6.26561  L
H-HC-0.029500        0    -8.69503   3.55341   4.83946  L
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H-HA-0.169900        0    -10.57194   0.66665   6.3582   L
H-HA-0.169900        0    -8.91634   2.43187   2.78988  L
H-HA-0.165600        0    -11.23146  -1.34384   5.04723  L
H-HA-0.165600        0    -9.49599   0.36402   1.50422  L
H-HO-0.399200        0    -11.65435  -1.95415   2.76817  L
N-N--0.516300        0    -11.97009   2.69656   7.56134  L
C-CT-0.038100        -1   -13.20095   2.1322    8.09181  L
C-C-0.536600         0    -14.39527   3.09952   8.26835  L
O-O--0.581900        0    -15.53443   2.61446   8.31202  L
C-CT--0.030300       0    -12.87493   1.54008   9.48701  L
C-C-0.799400         0    -12.18369   0.17181   9.45643  L
O-O2--0.801400       0    -12.71421  -0.73435   8.7748   L
O-O2--0.801400       0    -11.17591  -0.049     10.15836  L
H-H-0.293600         0    -11.13919   2.73032   8.14437  L
H-H1-0.088000        0    -13.53024   1.32974   7.43138  L
H-HC--0.012200       0    -13.80404   1.41051   10.044   L
H-HC--0.012200       0    -12.27074   2.25225   10.04977  L
N-N--0.415700        0    -14.14392   4.40468   8.47051  L
C-CT--0.149000       -1   -15.08374   5.44907   8.90591  L
H-H-0.271900         0    -13.18844   4.69974   8.28587  L
H-H1-0.097600        0    -15.99049   5.39939   8.30087  L
H-H1-0.097600        0    -14.62169   6.42954   8.77835  L
H-H1-0.097600        0    -15.34193   5.30039   9.95477  L
C-CT--0.366200       -1   -19.82642  -0.93195  -1.27661  L
C-C-0.597200         0    -18.8225  -0.60123  -0.16087  L
O-O--0.567900        0    -18.4266   0.55349  -0.06606  L
H-HC-0.112300        0    -20.68328  -1.45239  -0.85599  L
H-HC-0.112300        0    -19.33164  -1.5513   -2.02337  L
H-HC-0.112300        0    -20.1511  -0.00302  -1.74367  L
N-N--0.415700        0    -18.39839  -1.56098   0.6913   L
C-CT--0.058100       -1   -17.26974  -1.36151   1.6501   L
C-C-0.597300         0    -16.43236  -2.60399   1.9682   L
O-O--0.567900        0    -16.86114  -3.43229   2.77652  L
C-CT--0.007400       0    -17.70177  -0.6006    2.91451  L
C-CC-0.186800        0    -16.51243   0.11999   3.50608  L
N-NB--0.543200       0    -15.47268  -0.50317   4.18725  L
C-CW--0.220700       0    -16.17791   1.42919   3.30692  L
C-CR-0.163500        0    -14.50906   0.42189   4.34245  L
N-NA--0.279500       0    -14.9257   1.60538   3.86757  L
H-H-0.271900         0    -18.76068  -2.49328   0.57068  L
H-H1-0.136000        0    -16.60863  -0.65561   1.15294  L
H-HC-0.036700        0    -18.12645  -1.28723   3.64716  L
H-HC-0.036700        0    -18.45785   0.1421    2.65802  L
H-H4-0.186200        0    -16.74918   2.15345   2.74027  L
H-H-0.333900         0    -14.35166   2.44633   3.89833  L
H-H5-0.143500        0    -13.53933   0.24956   4.7957   L
N-N--0.254800        0    -15.23186  -2.73555   1.37347  L
C-CT--0.026600       -1   -14.28495  -3.76385   1.76978  L
C-C-0.589600         0    -13.59374  -3.45669   3.08864  L
O-O--0.574800        0    -13.19787  -2.31989   3.34757  L
C-CT--0.007000       0    -13.23557  -3.79831   0.66704  L
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C-CT-0.018900        0    -13.25585  -2.39838   0.05584  L
C-CT-0.019200        0    -14.69756  -1.946     0.26255  L
H-H1-0.064100        0    -14.7821  -4.73264   1.83312  L
H-HC-0.025300        0    -13.56271  -4.52603  -0.0592   L
H-HC-0.025300        0    -12.24502  -4.06475   1.03919  L
H-HC-0.021300        0    -12.98362  -2.40764  -0.99996  L
H-HC-0.021300        0    -12.58881  -1.73899   0.60928  L
H-H1-0.039100        0    -14.69941  -0.87808   0.48222  L
H-H1-0.039100        0    -15.27659  -2.14897  -0.63985  L
N-N--0.347900        0    -13.32492  -4.48937   3.88949  L
C-CT--0.263700       -1   -12.55814  -4.3329    5.13228  L
C-C-0.734100         0    -11.05174  -4.68628   4.95113  L
O-O--0.589400        0    -10.73562  -5.53048   4.11861  L
C-CT--0.000700       0    -13.28677  -4.99133   6.31671  L
C-CT-0.039000        0    -14.59832  -4.23671   6.65378  L
C-CT-0.048600        0    -14.3724  -2.86394   7.32539  L
N-N2--0.529500       0    -15.28204  -1.80689   6.82415  L
C-CA-0.807600        0    -15.68337  -0.71431   7.45972  L
N-N2--0.862700       0    -15.39079  -0.46434   8.69566  L
N-N2--0.862700       0    -16.35329   0.21804   6.85348  L
H-H-0.274700         0    -13.59377  -5.41074   3.56799  L
H-H1-0.156000        0    -12.52352  -3.27093   5.36638  L
H-HC-0.032700        0    -12.63841  -4.99186   7.19486  L
H-HC-0.032700        0    -13.52013  -6.02578   6.06141  L
H-HC-0.028500        0    -15.18852  -4.85186   7.33364  L
H-HC-0.028500        0    -15.18575  -4.10902   5.74332  L
H-H1-0.068700        0    -13.35009  -2.53684   7.14187  L
H-H1-0.068700        0    -14.48497  -2.98313   8.4045   L
H-H-0.345600         0    -15.47793  -1.80129   5.82812  L
H-H-0.447800         0    -15.61208   0.45534   9.03471  L
H-H-0.447800         0    -14.50462  -0.89403   8.96285  L
H-H-0.447800         0    -16.42332   1.12621   7.29652  L
H-H-0.447800         0    -16.39569   0.14462   5.84375  L
N-N--0.415700        0    -10.11843  -3.99184   5.63344  L
C-CT--0.003100       -1   -8.63332  -4.10585   5.50917  L
C-C-0.597300         0    -8.0375   -4.95939   6.63567  L
O-O--0.567900        0    -8.487    -4.88955   7.78131  L
C-CT--0.003600       0    -7.99432  -2.70989   5.48435  L
C-CT--0.064500       0    -6.46015  -2.79094   5.3935   L
C-C-0.695100         0    -5.86257  -1.46722   4.96834  L
O-O--0.608600        0    -6.10708  -1.02343   3.85952  L
N-N--0.940700        0    -5.05279  -0.82301   5.77443  L
H-H-0.271900         0    -10.45661  -3.31349   6.3063   L
H-H1-0.085000        0    -8.41597  -4.60418   4.57054  L
H-HC-0.017100        0    -8.27475  -2.1545    6.37764  L
H-HC-0.017100        0    -8.3806   -2.16309   4.6264   L
H-HC-0.035200        0    -6.17389  -3.53068   4.6468   L
H-HC-0.035200        0    -6.05069  -3.09201   6.35529  L
H-H-0.425100         0    -4.76537   0.11141   5.51249  L
H-H-0.425100         0    -4.72447  -1.2959    6.62749  L
N-N--0.415700        0    -6.9904   -5.72003   6.31166  L
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C-CT--0.001400       -1   -6.25049  -6.56545   7.24352  L
C-C-0.597300         0    -4.74715  -6.51613   6.94942  L
O-O--0.567900        0    -4.31088  -6.67073   5.80284  L
C-CT--0.015200       0    -6.74706  -8.02185   7.1607   L
C-CA--0.001100       0    -8.24664  -8.19165   6.99928  L
C-CA--0.190600       0    -9.08976  -8.36564   8.1161   L
C-CA--0.190600       0    -8.79807  -8.12464   5.70681  L
C-CA--0.234100       0    -10.48428  -8.4872    7.93491  L
C-CA--0.234100       0    -10.18543  -8.22135   5.53197  L
C-C-0.322600         0    -11.03274  -8.41882   6.63625  L
O-OH--0.557900       0    -12.36814  -8.54743   6.42705  L
H-H-0.271900         0    -6.71005  -5.74972   5.33578  L
H-H1-0.087600        0    -6.41772  -6.2007    8.25814  L
H-HC-0.029500        0    -6.41766  -8.55391   8.05383  L
H-HC-0.029500        0    -6.27001  -8.50536   6.30644  L
H-HA-0.169900        0    -8.66847  -8.39117   9.11049  L
H-HA-0.169900        0    -8.1596   -7.95518   4.84927  L
H-HA-0.165600        0    -11.1469  -8.6211    8.77524  L
H-HA-0.165600        0    -10.61007  -8.11026   4.55233  L
H-HO-0.399200        0    -12.51243  -8.63805   5.47274  L
N-N--0.516300        0    -3.94072  -6.3157    7.98929  L
C-CT-0.039700        -1   -2.49022  -6.24291   7.85811  L
C-C-0.536600         0    -1.80253  -7.61755   7.92014  L
O-O--0.581900        0    -2.01562  -8.40606   8.84098  L
C-CT-0.056000        0    -1.86978  -5.2644    8.86374  L
C-CT-0.013600        0    -2.12002  -3.80414   8.4552   L
C-C-0.805400         0    -3.59368  -3.37445   8.55908  L
O-O2--0.818800       0    -4.29712  -3.8676    9.47461  L
O-O2--0.818800       0    -4.02626  -2.5397    7.73362  L
H-H-0.293600         0    -4.34829  -6.0252    8.86998  L
H-H1-0.110500        0    -2.28348  -5.83739   6.87411  L
H-HC--0.017300       0    -0.78899  -5.41784   8.8699   L
H-HC--0.017300       0    -2.24192  -5.4587    9.87067  L
H-HC--0.042500       0    -1.7672   -3.66466   7.43146  L
H-HC--0.042500       0    -1.50357  -3.16955   9.092    L
N-N--0.415700        0    -0.92743  -7.89572   6.94739  L
C-CT--0.002400       -1   -0.17904  -9.15365   6.82146  L
C-C-0.597300         0     1.32634  -8.93595   6.99739  L
O-O--0.567900        0     1.85406  -7.81989   7.04126  L
C-CT--0.034300       0    -0.53225  -9.81381   5.46925  L
C-CA-0.011800        0     0.03443  -9.11497   4.24087  L
C-CA--0.125600       0    -0.67942  -8.0815    3.60835  L
C-CA--0.125600       0     1.30288  -9.47239   3.74931  L
C-CA--0.170400       0    -0.09551  -7.36381   2.54727  L
C-CA--0.170400       0     1.89049  -8.75478   2.69173  L
C-CA--0.107200       0     1.19119  -7.694     2.09357  L
H-H-0.271900         0    -0.7988   -7.18607   6.23093  L
H-H1-0.097800        0    -0.50582  -9.82934   7.61276  L
H-HC-0.029500        0    -1.61879  -9.86441   5.37677  L
H-HC-0.029500        0    -0.17032  -10.84223   5.47887  L
H-HA-0.133000        0    -1.65875  -7.79933   3.97149  L
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H-HA-0.133000        0     1.83163  -10.29404   4.20047  L
H-HA-0.143000        0    -0.61951  -6.52949   2.10251  L
H-HA-0.143000        0     2.87806  -9.01202   2.34195  L
H-HA-0.129700        0     1.63676  -7.12068   1.29403  L
N-N--0.415700        0     2.04831  -10.0475   7.11909  L
C-CT--0.024900       -1    3.49251  -10.01742   7.30737  L
C-C-0.597300         0     4.24804  -9.51582   6.05957  L
O-O--0.567900        0     4.11767  -10.06303   4.96684  L
C-CT-0.211700        0     4.02206  -11.40477   7.71325  L
O-OH--0.654600       0     3.766    -12.41415   6.74262  L
H-H-0.271900         0     1.55945  -10.92358   7.04064  L
H-H1-0.084300        0     3.70769  -9.33378   8.12953  L
H-H1-0.035200        0     3.56489  -11.69651   8.66037  L
H-H1-0.035200        0     5.09996  -11.33374   7.86801  L
H-HO-0.427500        0     3.0118   -12.93304   7.05099  L
N-N--0.347900        0     5.11173  -8.50883   6.21716  L
C-CT--0.263700       -1    6.00453  -7.97906   5.1617   L
C-C-0.734100         0     7.07826  -8.98016   4.6999   L
O-O--0.589400        0     7.131    -10.1235   5.15861  L
C-CT--0.000700       0     6.57485  -6.64224   5.68407  L
C-CT-0.039000        0     7.69322  -6.7749    6.73253  L
C-CT-0.048600        0     8.0245   -5.43905   7.41363  L
N-N2--0.529500       0     8.344    -4.35771   6.45572  L
C-CA-0.807600        0     7.5871   -3.3198    6.13939  L
N-N2--0.862700       0     6.37313  -3.2085    6.58492  L
N-N2--0.862700       0     8.02045  -2.35327   5.38876  L
H-H-0.274700         0     5.11069  -8.07303   7.12598  L
H-H1-0.156000        0     5.38436  -7.76067   4.28955  L
H-HC-0.032700        0     5.75374  -6.05975   6.10644  L
H-HC-0.032700        0     6.96817  -6.06878   4.85379  L
H-HC-0.028500        0     8.59453  -7.15328   6.25298  L
H-HC-0.028500        0     7.39081  -7.48476   7.503    L
H-H1-0.068700        0     8.88707  -5.59429   8.06372  L
H-H1-0.068700        0     7.18872  -5.15133   8.05292  L
H-H-0.345600         0     9.27731  -4.36084   6.05169  L
H-H-0.447800         0     5.83662  -2.36075   6.35585  L
H-H-0.447800         0     5.96231  -3.88187   7.18815  L
H-H-0.447800         0     7.36613  -1.57338   5.2872   L
H-H-0.447800         0     8.92344  -2.34829   4.94252  L
N-N--0.415700        0     7.95115  -8.53509   3.80346  L
C-CT--0.051800       -1    9.28451  -9.07953   3.53692  L
C-C-0.597300         0     10.21596  -7.88373   3.7315   L
O-O--0.567900        0     10.26333  -6.97007   2.91256  L
C-CT--0.110200       0     9.29936  -9.6944    2.12206  L
C-CT-0.353100        0     10.62257  -10.3571   1.68616  L
C-CT--0.412100       0     10.33283  -11.40992   0.61348  L
C-CT--0.412100       0     11.62099  -9.37607   1.07377  L
H-H-0.271900         0     7.77304  -7.61361   3.41003  L
H-H1-0.092200        0     9.53554  -9.85461   4.2636   L
H-HC-0.045700        0     9.00807  -8.94545   1.38429  L
H-HC-0.045700        0     8.53319  -10.46399   2.11692  L
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H-HC--0.036100       0     11.07903  -10.85274   2.54314  L
H-HC-0.100000        0     11.26304  -11.88869   0.30567  L
H-HC-0.100000        0     9.87291   -10.93887  -0.25743  L
H-HC-0.100000        0     9.66751   -12.17657   1.00768  L
H-HC-0.100000        0     12.50843  -9.91485   0.74373  L
H-HC-0.100000        0     11.92523  -8.62942   1.7993   L
H-HC-0.100000        0     11.17151  -8.87432   0.21814  L
N-N--0.415700        0     10.9021   -7.84487   4.86736  L
C-CT-0.014300        -1    12.18911  -7.1764    4.905    L
C-C-0.597300         0     13.21427  -8.24279   4.43518  L
O-O--0.567900        0     13.19795  -9.3384    4.99671  L
C-CT--0.204100       0     12.54452  -6.71658   6.32946  L
C-C-0.713000         0     11.74587  -5.53262   6.83445  L
O-O--0.593100        0     11.08468  -4.80587   6.10969  L
N-N--0.919100        0     11.78284  -5.29097   8.12334  L
H-H-0.271900         0     10.82237  -8.64767   5.4733   L
H-H1-0.104800        0     12.21882  -6.32526   4.2228   L
H-HC-0.079700        0     13.59577  -6.42468   6.34045  L
H-HC-0.079700        0     12.42473  -7.55319   7.01831  L
H-H-0.419600         0     11.30492  -4.46755   8.43621  L
H-H-0.419600         0     12.3682   -5.85041   8.72215  L
N-N--0.415700        0     14.04433  -7.99105   3.41199  L
C-CT--0.051800       -1    15.13879  -8.90628   3.03337  L
C-C-0.597300         0     16.35618  -8.70817   3.97496  L
O-O--0.567900        0     16.63406  -7.57782   4.37239  L
C-CT--0.110200       0     15.50682  -8.744     1.52425  L
C-CT-0.353100        0     16.51368  -9.7759    0.93408  L
C-CT--0.412100       0     16.00615  -11.21276   1.10244  L
C-CT--0.412100       -1    16.7944   -9.59751  -0.57832  L
H-H-0.271900         0     14.02093  -7.08889   2.96017  L
H-H1-0.092200        0     14.77899  -9.92372   3.18201  L
H-HC-0.045700        0     15.92027  -7.74747   1.37462  L
H-HC-0.045700        0     14.59006  -8.80145   0.93928  L
H-HC--0.036100       0     17.45953  -9.68187   1.46287  L
H-HC-0.100000        0     15.02696  -11.32179   0.63671  L
H-HC-0.100000        0     15.9421   -11.47391   2.15619  L
H-HC-0.100000        0     16.70612  -11.90434   0.63259  L
H-HC-0.100000        0     15.89474  -9.80158  -1.1549   L
H-HC-0.100000        0     17.58765  -10.27843  -0.88705  L
H-HC-0.100000        0     17.12792  -8.57508  -0.76004  L
N-N--0.516300        0     17.0766   -9.77801   4.34764  L
C-CT-0.039700        -1    18.33182  -9.66932   5.13007  L
C-C-0.536600         0     19.42149  -8.8644    4.36334  L
O-O--0.581900        0     19.35153  -8.71914   3.13975  L
C-CT-0.056000        0     18.85208  -11.0462   5.58567  L
C-CT-0.013600        0     18.54509  -11.30934   7.07047  L
C-C-0.805400         0     19.07633  -10.2078   8.00994  L
O-O2--0.818800       0     18.4857   -10.05116   9.09908  L
O-O2--0.818800       0     20.01068  -9.47768   7.59743  L
H-H-0.293600         0     16.8176   -10.68499   4.00174  L
H-H1-0.110500        0     18.1001   -9.06617   6.0085   L
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H-HC--0.017300       0     19.93251  -11.09791   5.44306  L
H-HC--0.017300       0     18.40461  -11.83461   4.97774  L
H-HC--0.042500       0     18.98587  -12.26848   7.35113  L
H-HC--0.042500       0     17.46127  -11.39371   7.18323  L
N-N--0.415700        0     20.39365  -8.26313   5.06762  L
C-CT--0.025200       -1    21.4057  -7.32713   4.51342  L
C-C-0.597300         0     20.79697  -6.04273   3.881    L
O-O--0.567900        0     21.54823  -5.26638   3.29498  L
H-H-0.271900         0     20.41322  -8.49224   6.06594  L
H-H1-0.069800        0     21.98135  -7.84081   3.74359  L
H-H1-0.069800        0     22.08675  -7.02603   5.30856  L
N-N--0.415700        0     19.47299  -5.78504   3.96707  L
C-CT--0.038900       0     18.74468  -4.86107   3.05563  L
C-C-0.597300         0     17.79053  -3.85921   3.74846  L
O-O--0.567900        0     16.96392  -4.20972   4.58824  L
C-CT-0.365400        0     17.93861  -5.66087   2.00997  L
O-OH--0.676100       0     18.70123  -6.68155   1.40625  L
C-CT--0.243800       0     17.47095  -4.79332   0.83951  L
H-H-0.271900         0     18.91245  -6.45145   4.48282  L
H-H1-0.100700        0     19.48472  -4.28334   2.50327  L
H-H1-0.004300        0     17.06492  -6.10065   2.48413  L
H-HC-0.064200        0     16.81751  -3.99663   1.18567  L
H-HC-0.064200        0     16.91784  -5.41356   0.13396  L
H-HC-0.064200        0     18.33378  -4.36328   0.33024  L
H-HO-0.410200        0     18.93109  -7.3508    2.0787   L
N-N--0.415700        0     17.84503  -2.58153   3.34383  L
C-CT--0.087500       -1    16.94633  -1.47472   3.76447  L
C-C-0.597300         0     15.58029  -1.58978   3.05059  L
O-O--0.567900        0     15.53053  -1.58912   1.82399  L
C-CT-0.298500        0     17.55218  -0.10367   3.37725  L
C-CT--0.319200       -1    16.6951   1.0997    3.86414  L
C-CT--0.319200       -1    19.0001  -0.02482   3.89442  L
H-H-0.271900         0     18.52935  -2.37441   2.63178  L
H-H1-0.096900        0     16.8043  -1.51598   4.84368  L
H-HC--0.029700       0     17.60955  -0.0393    2.29032  L
H-HC-0.079100        0     16.56608   1.05846   4.94473  L
H-HC-0.079100        0     15.72571   1.10812   3.36659  L
H-HC-0.079100        0     17.22214   2.01667   3.60578  L
H-HC-0.079100        0     19.02713  -0.21238   4.96799  L
H-HC-0.079100        0     19.3986   0.97163   3.70093  L
H-HC-0.079100        0     19.64268  -0.7402    3.38179  L
N-N--0.415700        0     14.45891  -1.69543   3.78257  L
C-CT--0.023700       -1    13.15109  -2.11101   3.20943  L
C-C-0.597300         0     11.88903  -1.46048   3.85601  L
O-O--0.567900        0     10.77143  -1.98135   3.75574  L
C-CT-0.034200        0     13.02582  -3.64305   3.42345  L
C-CT-0.001800        0     14.09981  -4.55773   2.8123   L
S-S--0.273700        0     13.60964  -5.42278   1.29674  L
C-CT--0.053600       0     13.71745  -4.05694   0.1158   L
H-H-0.271900         0     14.60024  -1.78465   4.77618  L
H-H1-0.088000        0     13.11821  -1.89805   2.14031  L
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 H-HC-0.024100        0     12.0607  -3.98835   3.05014  L
 H-HC-0.024100        0     13.03195  -3.82003   4.49955  L
 H-H1-0.044000        0     14.34506  -5.3143    3.55683  L
 H-H1-0.044000        0     15.01822  -4.01289   2.62221  L
 H-H1-0.068400        0     14.71771  -3.62402   0.13689  L
 H-H1-0.068400        0     12.9878  -3.28913   0.36848  L
 H-H1-0.068400        0     13.51095  -4.43687  -0.8821   L
 N-N--0.415700        0     12.03464  -0.31228   4.52381  L
 C-CT--0.024900       -1    10.92758   0.61778   4.83902  L
 C-C-0.597300         0     11.02082   1.73526   3.80464  L
 O-O--0.567900        0     12.12161   2.24208   3.58093  L
 C-CT-0.211700        0     11.05799   1.13335   6.2702   L
 O-OH--0.654600       0     10.13246   2.16007   6.55832  L
 H-H-0.271900         0     12.95824   0.09336   4.47487  L
 H-H1-0.084300        0     9.96383   0.11907   4.73401  L
 H-H1-0.035200        0     12.06494   1.5178    6.41478  L
 H-H1-0.035200        0     10.89728   0.30346   6.95947  L
 H-HO-0.427500        0     9.24129   1.89403   6.23071  L
 N-N--0.347900        0     9.92785   2.06967   3.10445  L
 C-CT--0.240000       -1    9.9923    2.98092   1.9464   L
 C-C-0.734100         0     10.58212   4.34826   2.36081  L
 O-O--0.589400        0     11.58517   4.74309   1.77402  L
 C-CT--0.009400       0     8.62292   3.05653   1.21759  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.66894   3.54599  -0.25182  H
 C-CT--0.047900       0     7.43632   3.06566  -1.04464  H
 C-CT--0.014300       0     7.28324   3.74296  -2.40447  H
 N-N3--0.385400       0     6.01239   3.31311  -3.11772  H
 H-H-0.274700         0     9.04017   1.6498    3.363    L
 H-H1-0.142600        0     10.70804   2.55583   1.24102  L
 H-HC-0.036200        0     7.94905   3.70758   1.77489  L
 H-HC-0.036200        0     8.19211   2.05312   1.21803  L
 H-HC-0.010300        0     9.58112   3.16662  -0.72141  H
 H-HC-0.010300        0     8.7203    4.6397   -0.24076  H
 H-HC-0.062100        0     6.51678   3.26078  -0.49253  H
 H-HC-0.062100        0     7.48998   1.9836   -1.19305  H
 H-HP-0.113500        0     8.10072   3.54643  -3.1029   H
 H-HP-0.113500        0     7.19966   4.826    -2.29763  H
 H-H-0.340000         0     6.1727    2.59511  -3.83756  H
 H-H-0.340000         0     5.61189   4.08754  -3.68682  H
 H-H-0.340000         0     5.24486   2.96628  -2.48607  H
 N-N--0.347900        0     10.11115   4.95493   3.47332  L
 C-CT--0.263700       -1    10.67692   6.13567   4.21628  L
 C-C-0.734100         0     12.02025   5.91293   4.89854  L
 O-O--0.589400        0     12.37161   6.61214   5.84556  L
 C-CT--0.000700       0     9.60284   6.67474   5.1923   L
 C-CT-0.039000        0     8.31418   7.11756   4.4701   L
 C-CT-0.048600        0     7.47907   8.11642   5.28619  L
 N-N2--0.529500       0     6.54616   7.49387   6.25619  L
 C-CA-0.807600        0     5.29813   7.88721   6.46914  L
 N-N2--0.862700       0     4.6765    8.7012    5.67909  L
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N-N2--0.862700       0     4.61938   7.48483   7.49856  L
H-H-0.274700         0     9.28708   4.50974   3.85165  L
H-H1-0.156000        0     10.88171   6.92178   3.48444  L
H-HC-0.032700        0     10.0161   7.54421   5.70614  L
H-HC-0.032700        0     9.36108   5.91781   5.94021  L
H-HC-0.028500        0     7.70419   6.25264   4.20395  L
H-HC-0.028500        0     8.59972   7.6214    3.54573  L
H-H1-0.068700        0     6.91999   8.71962   4.57246  L
H-H1-0.068700        0     8.14314   8.80458   5.81128  L
H-H-0.345600         0     6.88762   6.81006   6.90687  L
H-H-0.447800         0     3.70391   8.92198   5.87465  L
H-H-0.447800         0     4.99359   8.76572   4.7206   L
H-H-0.447800         0     3.65992   7.82604   7.55623  L
H-H-0.447800         0     4.93223   6.73891   8.10764  L
N-N--0.347900        0     12.76822   4.93191   4.40482  L
C-CT--0.240000       -1    14.15542   4.6386    4.74336  L
C-C-0.734100         0     15.0158   4.28763   3.5002   L
O-O--0.589400        0     16.23341   4.28322   3.62195  L
C-CT--0.009400       0     14.25763   3.57461   5.85951  L
C-CT-0.018700        0     13.44529   3.99696   7.09734  L
C-CT--0.047900       0     13.61305   3.12482   8.34317  L
C-CT--0.014300       0     12.55933   3.61842   9.34684  L
N-N3--0.385400       0     12.62898   2.91019   10.64764  L
H-H-0.274700         0     12.33909   4.41518   3.65166  L
H-H1-0.142600        0     14.60531   5.55599   5.13011  L
H-HC-0.036200        0     15.30597   3.4665    6.14283  L
H-HC-0.036200        0     13.89971   2.61398   5.49073  L
H-HC-0.010300        0     12.38746   3.99174   6.83215  L
H-HC-0.010300        0     13.73209   5.01385   7.36912  L
H-HC-0.062100        0     14.62126   3.25222   8.74193  L
H-HC-0.062100        0     13.44155   2.07723   8.09534  L
H-HP-0.113500        0     11.56847   3.48433   8.89685  L
H-HP-0.113500        0     12.70504   4.6937    9.49664  L
H-H-0.340000         0     12.46764   1.92034   10.51982  L
H-H-0.340000         0     11.9194   3.27074   11.2746  L
H-H-0.340000         0     13.53532   3.04753   11.0761  L
N-N--0.415700        0     14.41887   4.01223   2.32682  L
C-CT--0.051800       -1    15.05974   3.56705   1.06165  L
C-C-0.597300         0     15.26922   4.6703    0.05743  L
O-O--0.567900        0     16.23155   4.643    -0.70733  L
C-CT--0.110200       0     14.20107   2.41063   0.50668  L
C-CT-0.353100        0     14.72168   1.73967  -0.77949  L
C-CT--0.412100       0     16.11401   1.13173  -0.60591  L
C-CT--0.412100       0     13.76266   0.61585  -1.18128  L
H-H-0.271900         0     13.41109   4.0806    2.31358  L
H-H1-0.092200        0     16.04859   3.17413   1.30351  L
H-HC-0.045700        0     13.1989   2.79369   0.30776  L
H-HC-0.045700        0     14.11599   1.64568   1.2805   L
H-HC--0.036100       0     14.74787   2.46997  -1.5876   L
H-HC-0.100000        0     16.11753   0.42743   0.22488  L
H-HC-0.100000        0     16.84466   1.91852  -0.42064  L
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H-HC-0.100000        0     16.4044   0.61096  -1.51798  L
H-HC-0.100000        0     14.09706   0.17057  -2.11812  L
H-HC-0.100000        0     12.76036   1.01839  -1.32268  L
H-HC-0.100000        0     13.74126  -0.15325  -0.40786  L
N-N--0.415700        0     14.38019   5.65064   0.07525  L
C-CT-0.014300        -1    14.6044   6.87333  -0.64871  L
C-C-0.597300         0     15.69161   7.77742   0.00257  L
O-O--0.567900        0     15.40662   8.86787   0.49055  L
C-CT--0.204100       0     13.24998   7.57569  -0.93191  L
C-C-0.713000         0     12.26304   7.7071    0.22656  L
O-O--0.593100        0     12.56397   7.54193   1.39918  L
N-N--0.919100        0     11.01095   7.97044  -0.08034  L
H-H-0.271900         0     13.63201   5.63574   0.75839  L
H-H1-0.104800        0     15.00925   6.61515  -1.62898  L
H-HC-0.079700        0     12.74553   7.01416  -1.71744  L
H-HC-0.079700        0     13.44525   8.57558  -1.31796  L
H-H-0.419600         0     10.37474   8.03027   0.69013  L
H-H-0.419600         0     10.68964   8.09305  -1.03776  L
N-N--0.415700        0     16.95923   7.33056  -0.04865  L
C-CT--0.149000       -1    18.16195   8.01488   0.44647  L
H-H-0.271900         0     17.0645   6.4028   -0.44648  L
H-H1-0.097600        0     18.09985   8.12232   1.53086  L
H-H1-0.097600        0     18.22905   9.00854  -0.00041  L
H-H1-0.097600        0     19.05299   7.44045   0.19012  L
C-CT--0.055800       0     2.92824   14.02687   4.27069  L
C-CT-0.000000        0     2.85907   13.19905   2.98667  L
O-OS--0.354800       0     4.17203   12.96967   2.48578  L
C-CT--0.202200       0     2.24529   11.83188   3.25991  L
O-OS--0.524600       0     1.52295   11.44775   2.08875  L
C-CT--0.067000       0     3.48065   10.99274   3.54558  L
O-OH--0.613900       0     3.1926    9.64247   3.30797  L
C-CT--0.006600       0     4.44093   11.5736   2.52154  L
N-N*--0.048400       0     5.87038   11.29905   2.84064  L
C-C-0.753800         0     6.5951    10.41202   2.03562  L
O-O--0.625200        0     6.05857   9.81155   1.10686  L
N-NC--0.758400       0     7.91561   10.19225   2.26528  L
C-CA-0.818500        0     8.48824   10.82056   3.26549  L
N-N2--0.953000       0     9.75841   10.57677   3.42272  L
C-CM--0.521500       0     7.80115   11.69186   4.15175  L
C-CM--0.005300       0     6.48466   11.91244   3.90398  L
H-H1-0.067900        0     1.91595   14.20919   4.63374  L
H-H1-0.067900        0     3.4853    13.48193   5.03202  L
H-H1-0.117400        0     2.23645   13.72958   2.26298  L
H-H1-0.061500        0     1.57871   11.88374   4.11908  L
H-H1-0.097200        0     3.82653   11.16767   4.56608  L
H-HO-0.418600        0     2.33945   9.65728   2.83358  L
H-H2-0.202900        0     4.16354   11.13293   1.56346  L
H-H-0.423400         0     10.16889   10.02118   2.69577  L
H-H-0.423400         0     10.28758   11.08096   4.10567  L
H-HA-0.192800        0     8.28496   12.19324   4.97313  L
H-H4-0.195800        0     5.90348   12.58841   4.52121  L
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 P-P-1.166200         0     0.24178   10.44621   2.10039  L
 O-O2--0.776000       0    -0.73851   10.85931   1.08103  L
 O-O2--0.776000       0    -0.17221   10.1456   3.49155  L
 O-OS--0.498900       0     0.96966   9.1352    1.55987  L
 C-CT-0.055800        0     1.58241   9.10426   0.28643  L    H-H1
1581  0.        0.
 C-CT-0.106500        0     2.27221   7.74947   0.08826  H
 O-OS--0.354800       0     3.13788   7.52148   1.19494  H
 C-CT-0.202200        0     1.31504   6.55991  -0.03265  H
 O-OH--0.654100       0     1.2722    6.0273   -1.34141  H
 C-CT-0.067000        0     1.88078   5.47421   0.95602  H
 O-OH--0.613900       0     2.47581   4.35888   0.36444  H
 C-CT-0.039400        0     2.95278   6.24667   1.78579  H
 N-N*--0.025100       0     2.60501   6.34691   3.19733  H
 C-CK-0.200600        0     1.48114   6.92228   3.76668  H
 N-NB--0.607300       0     1.33439   6.65684   5.03732  H
 C-CB-0.051500        0     2.39498   5.8296    5.3297   H
 C-CA-0.700900        0     2.70129   5.08663   6.48513  H
 N-N2--0.901900       0     1.95533   5.15476   7.62695  H
 N-NC--0.761500       0     3.82584   4.3584    6.50147  H
 C-CQ-0.587500        0     4.52007   4.26353   5.36112  H
 N-NC--0.699700       0     4.30712   4.85385   4.18968  H
 C-CB-0.305300        0     3.21182   5.62857   4.21627  H
 H-H1-0.067900        0     2.33088   9.89286   0.22995  L
 H-H1-0.067900        0     0.83362   9.26059  -0.49396  L
 H-H1-0.117400        0     2.85991   7.79893  -0.83986  H
 H-H1-0.061500        0     0.30326   6.84349   0.29043  H
 H-HO-0.437600        0     0.93968   6.68457  -1.99246  H
 H-H1-0.097200        0     1.07017   5.18479   1.63657  H
 H-HO-0.418600        0     3.93241   4.0423    0.90637  H
 H-H2-0.200700        0     3.90915   5.73383   1.77682  H
 H-H5-0.155300        0     0.79778   7.52737   3.18344  H
 H-H-0.411500         0     1.93772   4.28218   8.16516  H
 H-H-0.411500         0     1.01374   5.51459   7.48888  H
 H-H5-0.047300        0     5.39619   3.62322   5.40533  H
 N-N3-0.149300        0    -0.48226   4.13397  -0.19757  H
 C-CT-0.053600        0     0.27384   3.03431   0.44383  H
 C-CT-0.065100        0    -0.48933   1.70633   0.25371  H
 C-CT--0.090300       0    -0.52544   0.79437   1.49013  H
 C-C-0.735400         0    -1.58909  -0.28959   1.33091  H
 O-O--0.613300        0    -1.33258  -1.46143   1.11985  H
 N-N--1.003100        0    -2.87955   0.1848    1.32551  H
 C-C-0.612300         0     1.64937   3.02321  -0.25165  H
 O-O--0.571300        0     1.68336   2.99814  -1.48048  H
 O-OS--0.421200       0     2.49526   1.98113   0.43256  H
 P-P-1.166200         0     3.87791   1.41316  -0.1002   H
 O-O2--0.776000       0     4.87969   1.43217   1.11684  H
 O-O2--0.776000       0     4.45855   2.04157  -1.33527  H
 O-OS--0.498900       0     3.74188  -0.1552   -0.29831  H
 C-CT-0.055800        0     2.99434  -0.61299  -1.43851  H
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 C-CT-0.106500        0     2.41606  -2.0086   -1.14477  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.40403  -2.94606  -0.71116  L
 C-CT-0.039400        0     3.27584  -3.1348    0.70065  L
 N-N*--0.025100       0     4.61471  -3.07241   1.3399   L
 C-CB-0.305300        0     5.37798  -4.17381   1.63758  L
 N-NC--0.699700       0     5.0244   -5.47863   1.46749  L
 C-CQ-0.587500        0     5.97814  -6.30618   1.85897  L
 N-NC--0.761500       0     7.17031  -6.01236   2.36066  L
 C-CA-0.700900        0     7.48908  -4.72212   2.47275  L
 N-N2--0.901900       0     8.72124  -4.52978   2.90827  L
 C-CB-0.051500        0     6.5687   -3.70429   2.12472  L
 N-NB--0.607300       0     6.58318  -2.30435   2.15108  L
 C-CK-0.200600        0     5.38743  -1.99102   1.70716  L
 C-CT-0.067000        0     2.22573  -2.1521    1.2275   L
 O-OH--0.613900       0     1.48723  -2.66398   2.32362  L
 C-CT-0.202200        0     1.37483  -1.97517  -0.03698  L
 O-OH--0.654100       0     0.46031  -3.05197  -0.21066  L
 H-H-0.199600         0    -1.71688   3.69349  -1.33041  H
 H-H-0.199600         0     0.12261   4.6671   -0.82105  H
 H-H-0.199600         0    -0.87727   4.76564   0.49569  H
 H-HP-0.101500        0     0.40128   3.23244   1.51578  H
 H-HC-0.005000        0    -0.09149   1.17033  -0.6152   H
 H-HC-0.005000        0    -1.5184    1.96961  -0.00621  H
 H-HC-0.033100        0    -0.76853   1.39414   2.3783   H
 H-HC-0.033100        0     0.43415   0.31218   1.67571  H
 H-H-0.442900         0    -3.61158  -0.49107   1.48154  H
 H-H-0.442900         0    -3.04138   1.0755    1.80201  H
 H-H1-0.067900        0     3.65878  -0.66956  -2.30621  H
 H-H1-0.067900        0     2.17432   0.0702   -1.66091  H
 H-H1-0.117400        0     1.93083  -2.35683  -2.05636  L
 H-H2-0.200700        0     2.86175  -4.1289    0.87734  L
 H-H5-0.047300        0     5.75172  -7.3576    1.75976  L
 H-H-0.411500         0     9.09304  -3.59488   2.96359  L
 H-H-0.411500         0     9.30666  -5.35771   2.96528  L
 H-H5-0.155300        0     5.04988  -0.96845   1.604    L
 H-H1-0.097200        0     2.67711  -1.20011   1.50269  L
 H-HO-0.418600        0     2.05502  -2.68771   3.11938  L
 H-H1-0.061500        0     0.84893  -1.02321  -0.04542  L
 H-HO-0.437600        0    -0.29254  -2.79778   0.36501  L
 O-OW--0.834000       0    -10.32525  -2.14299   11.54545  L
 H-HW-0.417000        0    -10.62485  -1.28976   11.14986  L
 H-HW-0.417000        0    -10.62158  -2.78839   10.87938  L
 O-OW--0.834000       0    -10.31797  -3.88727   9.45477  L
 H-HW-0.417000        0    -10.574   -3.23393   8.77601  L
 H-HW-0.417000        0    -9.68858  -4.45095   8.96506  L
 O-OW--0.834000       0    -10.75945  -1.95009   7.63971  L
 H-HW-0.417000        0    -11.55357  -1.546     8.07365  L
 H-HW-0.417000        0    -10.11505  -1.23964   7.72904  L
 O-OW--0.834000       0     4.89157   3.90993   1.1888   H
 H-HW-0.417000        0     5.35506   4.49997   0.56327  H
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H-HW-0.417000        0     5.07842   2.43726   1.22237  H
O-OW--0.834000       0     6.20995   2.6873    3.39366  H
H-HW-0.417000        0     5.51384   2.03627   3.21607  H
H-HW-0.417000        0     5.7405    3.52446   3.19862  H
O-OW--0.834000       0     6.52262   2.07489  -5.575    L
H-HW-0.417000        0     7.46017   1.90816  -5.79682  L
H-HW-0.417000        0     6.25062   2.71817  -6.2392   L
O-OW--0.834000       0     5.15464   5.00979   8.82405  L
H-HW-0.417000        0     4.67221   4.65039   8.04985  L
H-HW-0.417000        0     4.61437   4.70152   9.55866  L
O-OW--0.834000       0     7.80033   1.43769   5.37997  H
H-HW-0.417000        0     7.19177   1.95073   4.81295  H
H-HW-0.417000        0     7.15956   0.74439   5.70267  H
O-OW--0.834000       0     5.21673   7.82849   2.96918  H
H-HW-0.417000        0     4.33158   8.26333   2.94776  H
H-HW-0.417000        0     5.44137   8.00041   2.0339   H
O-OW--0.834000       0     5.82381   15.07514   3.16856  L
H-HW-0.417000        0     5.25549   14.32757   2.93154  L
H-HW-0.417000        0     5.20303   15.77797   3.3637   L
O-OW--0.834000       0    -4.26584   2.12689   5.52571  L
H-HW-0.417000        0    -4.09351   2.03095   6.46673  L
H-HW-0.417000        0    -4.73985   3.00124   5.5038   L
O-OW--0.834000       0     0.30053   1.77872   12.18022  L
H-HW-0.417000        0    -0.05226   1.46848   13.03589  L
H-HW-0.417000        0    -0.03711   2.67929   12.16165  L
O-OW--0.834000       0    -1.97944   9.69198   5.63156  L
H-HW-0.417000        0    -1.86611   8.80316   6.02385  L
H-HW-0.417000        0    -1.43326   9.66814   4.82127  L
O-OW--0.834000       0     2.10143   8.68198   6.85185  L
H-HW-0.417000        0     1.60395   8.02565   6.32931  L
H-HW-0.417000        0     1.56639   9.49464   6.70562  L
O-OW--0.834000       0    -4.68122   9.0735    5.60907  L
H-HW-0.417000        0    -4.64395   8.17623   5.99893  L
H-HW-0.417000        0    -3.76878   9.39545   5.70812  L
O-OW--0.834000       0    -2.20796   7.29597   7.013    L
H-HW-0.417000        0    -3.091     6.91269   6.80506  L
H-HW-0.417000        0    -2.03566   6.96923   7.91184  L
O-OW--0.834000       0     0.54165   10.69723   6.0468   L
H-HW-0.417000        0     0.51877   10.64656   5.06793  L
H-HW-0.417000        0    -0.40065   10.60935   6.25894  L
N-N                  0     6.81899   7.81006  -0.84143  H
H-H                  0     6.77332   8.64695  -1.39955  H
H-H                  0     7.45297   7.77569  -0.05614  H
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**IC**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.76832 | -11.37122 | -5.65126 | L |
| C-C-0.597200 | 0 | -12.07642 | -10.349 | -6.52345 | L |
| O-O--0.567900 | 0 | -11.6932 | -10.68593 | -7.63485 | L |
| H-HC-0.112300 | 0 | -12.16473 | -11.54676 | -4.76367 | L |
| H-HC-0.112300 | 0 | -12.86576 | -12.29841 | -6.21397 | L |
| H-HC-0.112300 | 0 | -13.75503 | -11.00089 | -5.38208 | L |
| N-N--0.415700 | 0 | -11.88598 | -9.13549 | -5.99651 | L |
| C-CT--0.058100 | -1 | -11.01014 | -8.10892 | -6.58196 | L |
| C-C-0.597300 | 0 | -9.97536 | -7.62336 | -5.56139 | L |
| O-O--0.567900 | 0 | -10.24496 | -7.57255 | -4.355 | L |
| C-CT--0.007400 | 0 | -11.80204 | -6.98477 | -7.24562 | L |
| C-CC-0.186800 | 0 | -11.18978 | -6.47776 | -8.5259 | L |
| N-NB--0.543200 | 0 | -11.58715 | -6.84616 | -9.81076 | L |
| C-CW--0.220700 | 0 | -10.30621 | -5.445 | -8.61201 | L |
| C-CR-0.163500 | 0 | -10.98746 | -5.97727 | -10.63786 | L |
| N-NA--0.279500 | 0 | -10.21547 | -5.12288 | -9.94789 | L |
| H-H-0.271900 | 0 | -12.25541 | -8.94419 | -5.08111 | L |
| H-H1-0.136000 | 0 | -10.44972 | -8.59351 | -7.38345 | L |
| H-HC-0.036700 | 0 | -11.86138 | -6.15157 | -6.55492 | L |
| H-HC-0.036700 | 0 | -12.81377 | -7.32468 | -7.47127 | L |
| H-H4-0.186200 | 0 | -9.8766 | -4.89736 | -7.78822 | L |
| H-H-0.333900 | 0 | -9.8535 | -4.23997 | -10.32879 | L |
| H-H5-0.143500 | 0 | -11.16405 | -5.91954 | -11.70252 | L |
| N-N--0.415700 | 0 | -8.78155 | -7.29221 | -6.04742 | L |
| C-CT--0.038900 | -1 | -7.61226 | -6.81795 | -5.28581 | L |
| C-C-0.597300 | 0 | -6.83198 | -5.73124 | -6.06344 | L |
| O-O--0.567900 | 0 | -7.17603 | -5.40017 | -7.1976 | L |
| C-CT-0.365400 | 0 | -6.63676 | -7.96791 | -4.95841 | L |
| O-OH--0.676100 | 0 | -6.37163 | -8.73244 | -6.09577 | L |
| C-CT--0.243800 | -1 | -7.15495 | -8.92282 | -3.89972 | L |
| H-H-0.271900 | 0 | -8.63571 | -7.47153 | -7.03501 | L |
| H-H1-0.100700 | 0 | -7.92394 | -6.40302 | -4.33508 | L |
| H-H1-0.004300 | 0 | -5.69813 | -7.55589 | -4.58772 | L |
| H-HC-0.064200 | 0 | -7.41507 | -8.36865 | -2.99778 | L |
| H-HC-0.064200 | 0 | -6.38475 | -9.65345 | -3.65763 | L |
| H-HC-0.064200 | 0 | -8.04065 | -9.44022 | -4.26936 | L |
| H-HO-0.410200 | 0 | -5.66569 | -9.37039 | -5.90216 | L |
| N-N--0.347900 | 0 | -5.75086 | -5.16997 | -5.48732 | L |
| C-CT--0.263700 | -1 | -4.75198 | -4.32809 | -6.19631 | L |
| C-C-0.734100 | 0 | -3.34685 | -4.44083 | -5.61458 | L |
| O-O--0.589400 | 0 | -3.22425 | -4.70526 | -4.42517 | L |
| C-CT--0.000700 | 0 | -5.21765 | -2.86357 | -6.29022 | L |
| C-CT-0.039000 | 0 | -4.98456 | -1.98777 | -5.04809 | L |
| C-CT-0.048600 | 0 | -5.79988 | -2.34017 | -3.80597 | L |
| N-N2--0.529500 | 0 | -5.19664 | -3.39846 | -2.99092 | L |
| C-CA-0.807600 | 0 | -5.20813 | -3.49066 | -1.68106 | L |
| N-N2--0.862700 | 0 | -5.92281 | -2.73428 | -0.90196 | L |
| N-N2--0.862700 | 0 | -4.44847 | -4.38587 | -1.13423 | L |
| H-H-0.274700 | 0 | -5.52472 | -5.48675 | -4.55654 | L |
| H-H1-0.156000 | 0 | -4.70523 | -4.72089 | -7.20864 | L |

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 H-HC-0.032700        0    -6.2747   -2.83075  -6.55932  L
 H-HC-0.032700        0    -4.6715   -2.40094  -7.11343  L
 H-HC-0.028500        0    -5.27187  -0.98109  -5.31898  L
 H-HC-0.028500        0    -3.92832  -1.95176  -4.79943  L
 H-H1-0.068700        0    -6.802    -2.63067  -4.11589  L
 H-H1-0.068700        0    -5.85601  -1.43429  -3.20079  L
 H-H-0.345600         0    -4.54238  -4.01409  -3.4506   L
 H-H-0.447800         0    -5.9652   -2.86467   0.0981   L
 H-H-0.447800         0    -6.67073  -2.14861  -1.29764  L
 H-H-0.447800         0    -4.16936  -4.24796  -0.16883  L
 H-H-0.447800         0    -3.99552  -5.08378  -1.71562  L
 N-N--0.415700        0    -2.29414  -4.13077  -6.36607  L
 C-CT--0.002400      -1    -1.04731  -3.6174   -5.76959  L
 C-C-0.597300         0    -1.12798  -2.09043  -5.73653  L
 O-O--0.567900        0    -1.17502  -1.49267  -6.81472  L
 C-CT--0.034300       0     0.16821  -4.10937  -6.56287  L
 C-CA-0.011800        0     1.48449  -3.53462  -6.06783  L
 C-CA--0.125600       0     1.96307  -3.84142  -4.77788  L
 C-CA--0.125600       0     2.23219  -2.68042  -6.89906  L
 C-CA--0.170400       0     3.17246  -3.28114  -4.32481  L
 C-CA--0.170400       0     3.4393   -2.12363  -6.44746  L
 C-CA--0.107200       0     3.89979  -2.4082   -5.15315  L
 H-H-0.271900         0    -2.49189  -3.95709  -7.34757  L
 H-H1-0.097800        0    -0.93419  -4.00194  -4.75738  L
 H-HC-0.029500        0     0.03363  -3.84946  -7.6143   L
 H-HC-0.029500        0     0.21624  -5.1966   -6.49045  L
 H-HA-0.133000        0     1.40219  -4.50238  -4.13177  L
 H-HA-0.133000        0     1.87638  -2.4406   -7.88764  L
 H-HA-0.143000        0     3.54189  -3.51372  -3.3372   L
 H-HA-0.143000        0     4.00335  -1.46173  -7.08929  L
 H-HA-0.129700        0     4.81049  -1.94371  -4.80337  L
 N-N--0.254800        0    -1.20989  -1.46493  -4.54662  L
 C-CT--0.026600       0    -1.24736  -0.01942  -4.41566  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.14595   0.54035  -4.05081  H
 O-O--0.574800        0     0.65021   0.30068  -2.96581  H
 C-CT--0.007000       0    -2.25379   0.21957  -3.28827  L
 C-CT-0.018900        0    -2.03432  -0.96506  -2.34404  L
 C-CT-0.019200        0    -1.50267  -2.07634  -3.25085  L
 H-H1-0.064100        0    -1.61459   0.43108  -5.32411  L
 H-HC-0.025300        0    -3.26717   0.18935  -3.6898   L
 H-HC-0.025300        0    -2.07698   1.16522  -2.78352  L
 H-HC-0.021300        0    -2.96437  -1.25652  -1.85473  L
 H-HC-0.021300        0    -1.28267  -0.7187   -1.59773  L
 H-H1-0.039100        0    -0.60067  -2.51209  -2.81968  L
 H-H1-0.039100        0    -2.27257  -2.83416  -3.34506  L
 N-N--0.254800        0     0.78105   1.36105  -4.94471  H
 C-CT--0.026600       0     2.04495   1.95498  -4.55476  H
 C-C-0.589600         0     2.05281   3.4718   -4.74703  H
 O-O--0.574800        0     1.4968    4.01974  -5.68662  H
 C-CT--0.007000       0     3.03227   1.37303  -5.58144  H
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 C-CT-0.018900        0     2.20447   1.31875  -6.87557  H
 C-CT-0.019200        0     0.72725   1.2863   -6.412    H
 H-H1-0.064100        0     2.27305   1.70577  -3.51909  H
 H-HC-0.025300        0     3.33812   0.37993  -5.24802  H
 H-HC-0.025300        0     3.92535   1.99308  -5.68944  H
 H-HC-0.021300        0     2.45816   0.45409  -7.49018  H
 H-HC-0.021300        0     2.37269   2.21952  -7.46811  H
 H-H1-0.039100        0     0.2118    2.15299  -6.81226  H
 H-H1-0.039100        0     0.21717   0.38247  -6.73269  H
 N-N--0.415700        0     2.86983   4.05333  -3.81422  H
 C-CT-0.039700        0     3.30832   5.4415   -3.86272  H
 C-C-0.597300         0     4.2236    5.6398   -5.11754  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.26046   4.96962  -5.1818   L
 C-CT--0.003600       0     3.93182   5.65669  -2.46291  H
 C-CT-0.013600        0     4.9378    6.76862  -2.26811  H
 C-C-0.805400         0     5.498     6.77487  -0.85844  H
 O-O2--0.818800       0     5.66659   5.7582   -0.16665  H
 H-H-0.271900         0     2.68703   3.69556  -2.86653  H
 H-H1-0.110500        0     2.46301   6.13255  -3.96176  H
 H-HC--0.017300       0     3.09318   5.77274  -1.78268  H
 H-HC--0.017300       0     4.3726    4.73927  -2.07631  H
 H-HC--0.042500       0     4.50817   7.75418  -2.45655  H
 H-HC--0.042500       0     5.78545   6.64919  -2.95197  H
 N-N--0.254800        0     3.86977   6.47994  -6.13574  L
 C-CT--0.026600      -1     4.67823   6.73972  -7.35787  L
 C-C-0.589600         0     6.11197   7.20356  -7.0396   L
 O-O--0.574800        0     7.00344   7.05005  -7.87412  L
 C-CT--0.007000       0     3.88901   7.689    -8.2568   L
 C-CT-0.018900        0     2.64489   8.08265  -7.46262  L
 C-CT-0.019200        0     2.6004    7.19175  -6.22114  L
 H-H1-0.064100        0     4.76923   5.79563  -7.88907  L
 H-HC-0.025300        0     3.58926   7.16043  -9.16275  L
 H-HC-0.025300        0     4.47628   8.56442  -8.53011  L
 H-HC-0.021300        0     1.7551    7.9258   -8.07092  L
 H-HC-0.021300        0     2.70527   9.12812  -7.16362  L
 H-H1-0.039100        0     2.44065   7.80846  -5.33643  L
 H-H1-0.039100        0     1.78027   6.48024  -6.31952  L
 N-N--0.415700        0     6.38034   7.71316  -5.83067  L
 C-CT-0.014300       -1     7.73351   7.88463  -5.31354  L
 C-C-0.597300         0     8.51948   6.58444  -5.17663  L
 O-O--0.567900        0     8.36481   5.81713  -4.22457  L
 C-CT--0.204100       0     7.74399   8.70283  -4.00451  L
 C-C-0.713000         0     9.15244   8.98945  -3.49943  L
 O-O--0.593100        0     9.68501   8.34349  -2.6081   L
 N-N--0.919100        0     9.81327   9.97765  -4.04774  L
 H-H-0.271900         0     5.59466   7.95983  -5.22967  L
 H-H1-0.104800        0     8.26098   8.4973   -6.04721  L
 H-HC-0.079700        0     7.22022   8.17024  -3.22186  L
 H-HC-0.079700        0     7.23544   9.64866  -4.1724   L
 H-H-0.419600         0     10.71879   10.17388  -3.66764  L
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H-H-0.419600         0     9.35615   10.59936  -4.71263  L
N-N--0.415700        0     9.46223   6.42606  -6.09709  L
C-CT--0.025200       -1    10.69749   5.71422  -5.85221  L
C-C-0.597300         0     11.03156   4.72771  -6.97709  L
O-O--0.567900        0     11.4895   5.10425  -8.05085  L
H-H-0.271900         0     9.4001    7.00519  -6.92365  L
H-H1-0.069800        0     10.65345   5.17982  -4.90257  L
H-H1-0.069800        0     11.51085   6.43704  -5.79132  L
N-N--0.415700        0     10.80066   3.45368  -6.68574  L
C-CT--0.001400       -1    10.78148   2.26996  -7.55814  L
C-C-0.597300         0     9.74087   1.34189  -6.91518  L
O-O--0.567900        0     8.9783    1.77739  -6.0439   L
C-CT--0.015200       0     12.205    1.67475  -7.62884  L
C-CA--0.001100       0     12.64447   1.29906  -9.0295   L
C-CA--0.190600       0     13.07732   2.31255  -9.90716  L
C-CA--0.190600       0     12.64127  -0.04448  -9.45307  L
C-CA--0.234100       0     13.51382   1.98786  -11.20605  L
C-CA--0.234100       0     13.06602  -0.37183  -10.75525  L
C-C-0.322600         0     13.50538   0.64157  -11.63168  L
O-OH--0.557900       0     13.91221   0.32031  -12.88725  L
H-H-0.271900         0     10.3431   3.30326  -5.79803  L
H-H1-0.087600        0     10.4419   2.55288  -8.5561   L
H-HC-0.029500        0     12.29301   0.81163  -6.96801  L
H-HC-0.029500        0     12.92332   2.40969  -7.26101  L
H-HA-0.169900        0     13.06809   3.34468  -9.57767  L
H-HA-0.169900        0     12.31868  -0.83125  -8.78614  L
H-HA-0.165600        0     13.84344   2.76966  -11.87208  L
H-HA-0.165600        0     13.06224  -1.39581  -11.09655  L
H-HO-0.399200        0     14.2126   1.09311  -13.36537  L
N-N--0.415700        0     9.76622   0.05368  -7.21108  L
C-CT--0.051800       -1    9.32666  -0.95535  -6.25048  L
C-C-0.597300         0     10.47834  -1.90238  -5.96302  L
O-O--0.567900        0     11.44089  -2.00805  -6.72224  L
C-CT--0.110200       0     8.02997  -1.62259  -6.75573  L
C-CT-0.353100        0     8.11741  -2.38423  -8.09639  L
C-CT--0.412100       0     8.61115  -3.82399  -7.91932  L
C-CT--0.412100       0     6.72636  -2.44842  -8.72692  L
H-H-0.271900         0     10.35673  -0.23923  -7.97889  L
H-H1-0.092200        0     9.0974   -0.46444  -5.30837  L
H-HC-0.045700        0     7.29239  -0.82462  -6.85726  L
H-HC-0.045700        0     7.65158  -2.30089  -5.99203  L
H-HC--0.036100       0     8.77752  -1.86164  -8.78775  L
H-HC-0.100000        0     9.64646  -3.83166  -7.58743  L
H-HC-0.100000        0     8.56265  -4.34384  -8.87629  L
H-HC-0.100000        0     7.99144  -4.35094  -7.19453  L
H-HC-0.100000        0     6.0279   -2.9497   -8.06203  L
H-HC-0.100000        0     6.77085  -2.97564  -9.68093  L
H-HC-0.100000        0     6.3673   -1.4404   -8.91258  L
N-N--0.415700        0     10.40105  -2.54979  -4.81447  L
C-CT--0.058100       -1    11.47786  -3.36293  -4.26766  L
C-C-0.597300         0     10.96185  -4.75594  -3.93303  L
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 O-O--0.567900        0     9.7606   -5.01418  -3.93376  L
 C-CT--0.007400       0     12.06946  -2.62968  -3.04993  L
 C-CC-0.186800        0     11.06317  -2.2976   -1.9697   L
 N-NB--0.543200       0     10.66557  -3.14572  -0.93684  L
 C-CW--0.220700       0     10.34933  -1.13866  -1.88534  L
 C-CR-0.163500        0     9.72922  -2.47451  -0.24544  L
 N-NA--0.279500       0     9.50539  -1.2751   -0.80368  L
 H-H-0.271900         0     9.55332  -2.42863  -4.27289  L
 H-H1-0.136000        0     12.2653  -3.48367  -5.01389  L
 H-HC-0.036700        0     12.51979  -1.69768  -3.39438  L
 H-HC-0.036700        0     12.86762  -3.23132  -2.62058  L
 H-H4-0.186200        0     10.40076  -0.30929  -2.57726  L
 H-H-0.333900         0     8.76281  -0.64395  -0.52911  L
 H-H5-0.143500        0     9.19025  -2.85791   0.61188  L
 N-N--0.415700        0     11.86346  -5.68847  -3.64548  L
 C-CT--0.059700       -1    11.45201  -7.06252  -3.35597  L
 C-C-0.597300         0     10.53432  -7.19536  -2.11502  L
 O-O--0.567900        0     9.75309  -8.1402   -2.02393  L
 C-CT-0.130300        0     12.67339  -7.99436  -3.2769   L
 C-CT--0.043000       0     12.19261  -9.45917  -3.21285  L
 C-CT--0.320400       0     13.60838  -7.64397  -2.10408  L
 C-CT--0.066000       -1    13.2409  -10.44567  -3.70715  L
 H-H-0.271900         0     12.84424  -5.45814  -3.67935  L
 H-H1-0.086900        0     10.8616  -7.39481  -4.20758  L
 H-HC-0.018700        0     13.23403  -7.86351  -4.20464  L
 H-HC-0.023600        0     11.31669  -9.58441  -3.85023  L
 H-HC-0.023600        0     11.91251  -9.71991  -2.19133  L
 H-HC-0.088200        0     14.50161  -8.26381  -2.15162  L
 H-HC-0.088200        0     13.11192  -7.81701  -1.14863  L
 H-HC-0.088200        0     13.92512  -6.60359  -2.15862  L
 H-HC-0.018600        0     12.83138  -11.45552  -3.66944  L
 H-HC-0.018600        0     14.12804  -10.40375  -3.07563  L
 H-HC-0.018600        0     13.51613  -10.21443  -4.73677  L
 N-N--0.415700        0     10.56978  -6.23925  -1.17988  L
 C-CT--0.025200       -1    9.5501   -6.10447  -0.13813  L
 C-C-0.597300         0     8.15523  -5.95443  -0.74311  L
 O-O--0.567900        0     7.32534  -6.85616  -0.61617  L
 H-H-0.271900         0     11.20496  -5.46547  -1.30851  L
 H-H1-0.069800        0     9.77161  -5.24568   0.49087  L
 H-H1-0.069800        0     9.55598  -6.99709   0.48271  L
 N-N--0.415700        0     7.92247  -4.85343  -1.4695   L
 C-CT--0.058100       0     6.7245   -4.64819  -2.2995   L    H-HC
246   0.        0.
 C-C-0.597300         0     6.35593  -5.90031  -3.11152  L
 O-O--0.567900        0     5.17924  -6.24646  -3.18115  L
 C-CT--0.007400       0     6.91491  -3.47046  -3.26097  H
 C-CC-0.186800        0     6.87543  -2.05825  -2.76891  H
 N-NB--0.543200       0     7.57608  -1.12743  -3.49556  H
 C-CW--0.220700       0     6.10124  -1.42467  -1.83051  H
 C-CR-0.163500        0     7.18436   0.0418   -3.04642  H
 N-NA--0.279500       0     6.30427  -0.07749  -2.01702  H
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H-H-0.271900          0     8.69737  -4.21023  -1.58047  L
H-H1-0.136000         0     5.87117  -4.43273  -1.65344  L
H-HC-0.036700         0     6.13783  -3.56767  -4.02674  H
H-HC-0.036700         0     7.85096  -3.59154  -3.79925  H
H-H4-0.186200         0     5.41126  -1.76857  -1.0836   H
H-H-0.333900          0     5.74026   0.67666  -1.6164   H
H-H5-0.143500         0     7.53188   1.0043   -3.41373  H
N-N--0.415700         0     7.33765  -6.59999  -3.6954   L
C-CT-0.033700         -1    7.12563  -7.83829  -4.44733  L
C-C-0.597300          0     6.30703  -8.90589  -3.71697  L
O-O--0.567900         0     5.46455  -9.54745  -4.34367  L
C-CT--0.182500        0     8.43182  -8.38042  -5.03224  L
H-H-0.271900          0     8.27272  -6.21157  -3.64085  L
H-H1-0.082300         0     6.51485  -7.55704  -5.30338  L
H-HC-0.060300         0     8.98956  -7.57401  -5.50962  L
H-HC-0.060300         0     8.19901  -9.13504  -5.78482  L
H-HC-0.060300         0     9.03001  -8.85128  -4.2577   L
N-N--0.347900         0     6.48229  -9.0782   -2.40223  L
C-CT--0.240000        -1    5.58707  -9.93833  -1.61764  L
C-C-0.734100          0     4.1184   -9.46049  -1.65854  L
O-O--0.589400         0     3.23001  -10.29103  -1.82821  L
C-CT--0.009400        0     6.1105   -10.11097  -0.18161  L
C-CT-0.018700         0     5.21857  -11.06283   0.64161  L
C-CT--0.047900        0     5.84896  -11.39545   1.99833  L
C-CT--0.014300        0     4.87973  -12.17183   2.8982   L
N-N3--0.385400        0     5.4659   -12.40919   4.24256  L
H-H-0.274700          0     7.176    -8.49226  -1.94274  L
H-H1-0.142600         0     5.58351  -10.92306  -2.08857  L
H-HC-0.036200         0     6.1546   -9.13981   0.31149  L
H-HC-0.036200         0     7.12121  -10.52005  -0.23005  L
H-HC-0.010300         0     5.06244  -11.98966   0.08721  L
H-HC-0.010300         0     4.25169  -10.58808   0.8124   L
H-HC-0.062100         0     6.1109   -10.45928   2.48959  L
H-HC-0.062100         0     6.75093  -11.98743   1.83605  L
H-HP-0.113500         0     4.60856  -13.1168   2.41876  L
H-HP-0.113500         0     3.96941  -11.57209   3.00724  L
H-H-0.340000          0     4.74559  -12.67199   4.91131  L
H-H-0.340000          0     5.8359   -11.53101   4.60658  L
H-H-0.340000          0     6.20642  -13.09244   4.22789  L
N-N--0.415700         0     3.85067  -8.15745  -1.50355  L
C-CT--0.024900        -1    2.50471  -7.56374  -1.66572  L
C-C-0.597300          0     1.9441   -7.80242  -3.0784   L
O-O--0.567900         0     0.81181  -8.26713  -3.18192  L
C-CT-0.211700         0     2.49793  -6.06648  -1.31922  L
O-OH--0.654600        0     1.15808  -5.62187  -1.22674  L
H-H-0.271900          0     4.64682  -7.53584  -1.45007  L
H-H1-0.084300         0     1.83216  -8.06236  -0.96681  L
H-H1-0.035200         0     3.02463  -5.49464  -2.08255  L
H-H1-0.035200         0     2.98961  -5.92106  -0.35866  L
H-HO-0.427500         0     1.11037  -4.69862  -0.90841  L
N-N--0.415700         0     2.71852  -7.56453  -4.15484  L
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C-CT--0.059700       -1    2.37498  -7.96056  -5.54749  L
C-C-0.597300         0     1.93842  -9.44397  -5.54728  L
O-O--0.567900        0     0.80608  -9.73958  -5.90831  L
C-CT-0.130300        0     3.52437  -7.6835   -6.54764  L
C-CT--0.043000       0     3.92489  -6.19268  -6.5354   L
C-CT--0.320400       0     3.11283  -8.0985   -7.97281  L
C-CT--0.066000       0     5.15815  -5.86165  -7.38176  L
H-H-0.271900         0     3.62677  -7.14881  -3.97524  L
H-H1-0.086900        0     1.51063  -7.37371  -5.86051  L
H-HC-0.018700        0     4.39045  -8.27666  -6.26072  L
H-HC-0.023600        0     4.14804  -5.88487  -5.51676  L
H-HC-0.023600        0     3.08858  -5.59301  -6.89161  L
H-HC-0.088200        0     2.28784  -7.47756  -8.3238   L
H-HC-0.088200        0     2.80846  -9.14482  -8.00531  L
H-HC-0.088200        0     3.95243  -7.98459  -8.6579   L
H-HC-0.018600        0     4.90277  -5.86461  -8.44148  L
H-HC-0.018600        0     5.95479  -6.58091  -7.19835  L
H-HC-0.018600        0     5.51052  -4.87053  -7.10591  L
N-N--0.415700        0     2.78989  -10.37481  -5.09664  L
C-CT-0.021300        -1    2.54616  -11.82983  -5.12987  L
C-C-0.597300         0     1.31948  -12.32939  -4.3679   L
O-O--0.567900        0     0.75002  -13.34901  -4.74234  L
C-CT--0.123100       -1    3.84659  -12.594   -4.73595  L
S-SH--0.311900       0     5.19275  -12.24634  -5.90477  L
H-H-0.271900         0     3.70033  -10.05605  -4.78878  L
H-H1-0.112400        0     2.34004  -12.08984  -6.17013  L
H-H1-0.111200        0     3.63783  -13.66573  -4.75383  L
H-H1-0.111200        0     4.14622  -12.31076  -3.72619  L
H-HS-0.193300        0     5.37065  -10.96216  -5.56071  L
N-N--0.415700        0     0.90879  -11.63784  -3.30923  L
C-CT--0.051800       -1   -0.32701  -11.94128  -2.59346  L
C-C-0.597300         0    -1.55005  -11.26811  -3.2433   L
O-O--0.567900        0    -2.53762  -11.95308  -3.48443  L
C-CT--0.110200       0    -0.16917  -11.49482  -1.12869  L
C-CT-0.353100        0     0.84181  -12.34686  -0.33655  L
C-CT--0.412100       0     1.2003   -11.64447   0.97105  L
C-CT--0.412100       0     0.28528  -13.72982   0.00934  L
H-H-0.271900         0     1.46519  -10.8381  -3.03361  L
H-H1-0.092200        0    -0.51433  -13.01556  -2.61939  L
H-HC-0.045700        0    -1.13927  -11.55102  -0.63262  L
H-HC-0.045700        0     0.15002  -10.45086  -1.11701  L
H-HC--0.036100       0     1.75994  -12.47349  -0.90931  L
H-HC-0.100000        0     1.65774  -10.68463   0.73553  L
H-HC-0.100000        0     1.90422  -12.24909   1.53804  L
H-HC-0.100000        0     0.29924  -11.47421   1.56219  L
H-HC-0.100000        0     1.01382  -14.2897   0.59335  L
H-HC-0.100000        0     0.07934  -14.28655  -0.90454  L
H-HC-0.100000        0    -0.6389   -13.63057   0.57959  L
N-N--0.415700        0    -1.50573  -9.96125  -3.54765  L
C-CT-0.014300        -1   -2.60036  -9.24067  -4.22782  L
C-C-0.597300         0    -2.97417  -9.89651  -5.54278  L
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O-O--0.567900        0    -4.13023  -10.26739  -5.74829  L
C-CT--0.204100       0    -2.31633  -7.73821  -4.30474  L
C-C-0.713000         0    -2.51027  -7.07962  -2.94625  L
O-O--0.593100        0    -3.61214  -6.75579  -2.52661  L
N-N--0.919100        0    -1.45488  -6.86009  -2.20295  L
H-H-0.271900         0    -0.64268  -9.46319  -3.36388  L
H-H1-0.104800        0    -3.49223  -9.35712  -3.60678  L
H-HC-0.079700        0    -3.03348  -7.28879  -4.98957  L
H-HC-0.079700        0    -1.31413  -7.55046  -4.68745  L
H-H-0.419600         0    -1.57542  -6.37271  -1.33558  L
H-H-0.419600         0    -0.53939  -7.14493  -2.52442  L
N-N--0.415700        0    -1.96826  -10.1283  -6.37446  L
C-CT--0.002400      -1    -2.12661  -10.92807  -7.56792  L
C-C-0.597300         0    -2.33579  -12.42377  -7.34743  L
O-O--0.567900        0    -2.83255  -13.1095  -8.23525  L
C-CT--0.034300       0    -0.99136  -10.6414  -8.56637  L
C-CA-0.011800        0    -1.10732  -9.27718  -9.23009  L
C-CA--0.125600       0    -1.84233  -9.1431   -10.42398  L
C-CA--0.125600       0    -0.53963  -8.13192  -8.63824  L
C-CA--0.170400       0    -2.02308  -7.87658  -11.00881  L
C-CA--0.170400       0    -0.71077  -6.86626  -9.22926  L
C-CA--0.107200       0    -1.46098  -6.73679  -10.41013  L
H-H-0.271900         0    -1.03774  -9.81344  -6.12593  L
H-H1-0.097800        0    -3.04459  -10.59772  -8.05742  L
H-HC-0.029500        0    -1.0235   -11.39574  -9.35397  L
H-HC-0.029500        0    -0.02395  -10.74054  -8.07679  L
H-HA-0.133000        0    -2.29987  -10.00958  -10.87996  L
H-HA-0.133000        0     0.00676  -8.21799  -7.7147   L
H-HA-0.143000        0    -2.62028  -7.77195  -11.90527  L
H-HA-0.143000        0    -0.28927  -5.98632  -8.7697   L
H-HA-0.129700        0    -1.62318  -5.76229  -10.85098  L
N-N--0.415700        0    -2.00119  -12.92103  -6.16303  L
C-CT--0.025200      -1    -2.22994  -14.29668  -5.75471  L
C-C-0.597300         0    -3.69505  -14.69343  -5.61033  L
O-O--0.567900        0    -4.0661   -15.81773  -5.93377  L
H-H-0.271900         0    -1.62115  -12.28915  -5.47706  L
H-H1-0.069800        0    -1.74024  -14.46745  -4.79687  L
H-H1-0.069800        0    -1.77415  -14.96234  -6.48814  L
N-N--0.415700        0    -4.51529  -13.78052  -5.09225  L
C-CT--0.059700      -1    -5.97718  -13.91882  -5.02438  L
C-C-0.597300         0    -6.64614  -13.84699  -6.40047  L
O-O--0.567900        0    -7.67113  -14.49257  -6.61292  L
C-CT-0.130300        0    -6.5162   -12.88149  -3.98446  L
C-CT--0.043000       0    -6.1885   -13.39647  -2.54227  L
C-CT--0.320400      -1    -8.02797  -12.53558  -4.12481  L
C-CT--0.066000      -1    -5.49019  -12.41193  -1.57458  L
H-H-0.271900         0    -4.0902   -12.91148  -4.79189  L
H-H1-0.086900        0    -6.21314  -14.91672  -4.65257  L
H-HC-0.018700        0    -5.97091  -11.94985  -4.14464  L
H-HC-0.023600        0    -5.53818  -14.26981  -2.60535  L
H-HC-0.023600        0    -7.11043  -13.74005  -2.07135  L
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H-HC-0.088200        0    -8.21202  -12.042   -5.08121  L
H-HC-0.088200        0    -8.32872  -11.85819  -3.32565  L
H-HC-0.088200        0    -8.62595  -13.44629  -4.07553  L
H-HC-0.018600        0    -4.53513  -12.09657  -1.98531  L
H-HC-0.018600        0    -5.32512  -12.89746  -0.61265  L
H-HC-0.018600        0    -6.12361  -11.5364  -1.43222  L
N-N--0.415700        0    -6.04576  -13.10921  -7.33756  L
C-CT--0.149000       -1   -6.4547   -13.07715  -8.72997  L
H-H-0.271900         0    -5.19853  -12.63351  -7.07001  L
H-H1-0.097600        0    -6.74631  -14.07759  -9.05508  L
H-H1-0.097600        0    -5.62869  -12.72526  -9.34918  L
H-H1-0.097600        0    -7.30791  -12.4044  -8.84235  L
C-CT--0.366200       -1   -8.85774  -9.87656  -10.83288  L
C-C-0.597200         0    -8.09314  -9.21606  -9.75157  L
O-O--0.567900        0    -8.43915  -9.24823  -8.57832  L
H-HC-0.112300        0    -8.23001  -10.59832  -11.35    L
H-HC-0.112300        0    -9.23828  -9.12086  -11.51833  L
H-HC-0.112300        0    -9.70624  -10.39037  -10.37937  L
N-N--0.415700        0    -7.0266   -8.60103  -10.20593  L
C-CT-0.021300        -1   -6.21977  -7.75127  -9.38825  L
C-C-0.597300         0    -5.714    -6.58802  -10.24007  L
O-O--0.567900        0    -5.11582  -6.8316   -11.29173  L
C-CT--0.123100       0    -5.02639  -8.56086  -8.85804  L
S-SH--0.311900       0    -3.92856  -7.4958   -7.86596  L
H-H-0.271900         0    -6.8474   -8.60599  -11.19711  L
H-H1-0.112400        0    -6.79986  -7.36921  -8.54936  L
H-H1-0.111200        0    -4.46815  -8.9729   -9.69812  L
H-H1-0.111200        0    -5.3957   -9.38754  -8.25084  L
H-HS-0.193300        0    -3.43757  -6.78508  -8.89439  L
N-N--0.415700        0    -5.91567  -5.34635  -9.79604  L
C-CT-0.014300        -1   -5.44496  -4.17505  -10.5307  L
C-C-0.597300         0    -4.07455  -3.63733  -10.03344  L
O-O--0.567900        0    -3.48282  -4.12843  -9.06714  L
C-CT--0.204100       0    -6.56857  -3.1238   -10.62993  L
C-C-0.713000         0    -6.36837  -2.13445  -11.77679  L
O-O--0.593100        0    -5.53428  -2.32045  -12.65312  L
N-N--0.919100        0    -7.06712  -1.03417  -11.79998  L
H-H-0.271900         0    -6.43997  -5.22166  -8.93483  L
H-H1-0.104800        0    -5.25968  -4.49583  -11.5575  L
H-HC-0.079700        0    -6.66633  -2.58041  -9.69052  L
H-HC-0.079700        0    -7.50343  -3.64352  -10.82877  L
H-H-0.419600         0    -6.94307  -0.41969  -12.57501  L
H-H-0.419600         0    -7.84789  -0.90149  -11.14171  L
N-N--0.415700        0    -3.53821  -2.61805  -10.70443  L
C-CT--0.051800       -1   -2.35198  -1.85028  -10.33105  L
C-C-0.597300         0    -2.78609  -0.38315  -10.04402  L
O-O--0.567900        0    -3.17566   0.32156  -10.97243  L
C-CT--0.110200       0    -1.31437  -1.93893  -11.46898  L
C-CT-0.353100        0    -0.10144  -0.99935  -11.30526  L
C-CT--0.412100       0     0.72409  -1.3297   -10.06206  L
C-CT--0.412100       0     0.82138  -1.11408  -12.51888  L
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H-H-0.271900          0    -4.06788  -2.28569  -11.50704  L
H-H1-0.092200         0    -1.91341  -2.26023  -9.42085  L
H-HC-0.045700         0    -1.81369  -1.68205  -12.40527  L
H-HC-0.045700         0    -0.96605  -2.9696   -11.54667  L
H-HC--0.036100        0    -0.43556   0.03503  -11.23787  L
H-HC-0.100000         0     1.05166  -2.36816  -10.10386  L
H-HC-0.100000         0     0.12517  -1.16959  -9.16639  L
H-HC-0.100000         0     1.59143  -0.67243  -10.01213  L
H-HC-0.100000         0     1.20322  -2.1314   -12.60598  L
H-HC-0.100000         0     1.65141  -0.4173   -12.41155  L
H-HC-0.100000         0     0.26369  -0.86008  -13.42066  L
N-N--0.347900         0    -2.72726   0.09553  -8.78546  L
C-CT--0.263700        -1   -3.4502    1.30836  -8.31005  L
C-C-0.734100          0    -2.54325   2.35462  -7.6831   L
O-O--0.589400         0    -2.16681   2.23784  -6.5265   L
C-CT--0.000700        0    -4.54391   0.85303  -7.33172  L
C-CT-0.039000         0    -5.59908   1.93416  -7.05196  L
C-CT-0.048600         0    -6.34661   1.63274  -5.74904  L
N-N2--0.529500        0    -5.55785   2.04833  -4.57265  L
C-CA-0.807600         0    -5.94754   2.02785  -3.31678  L
N-N2--0.862700        0    -7.07796   1.5544   -2.91764  L
N-N2--0.862700        0    -5.19427   2.48548  -2.37875  L
H-H-0.274700          0    -2.30705  -0.5049   -8.08274  L
H-H1-0.156000         0    -3.95384   1.77489  -9.15928  L
H-HC-0.032700         0    -4.06368   0.55329  -6.40007  L
H-HC-0.032700         0    -5.06079  -0.01607  -7.7429   L
H-HC-0.028500         0    -6.31091   1.95216  -7.87875  L
H-HC-0.028500         0    -5.13565   2.91911  -6.97401  L
H-H1-0.068700         0    -6.60284   0.57563  -5.69929  L
H-H1-0.068700         0    -7.29094   2.16416  -5.75631  L
H-H-0.345600          0    -4.69845   2.5874   -4.70322  L
H-H-0.447800          0    -7.32966   1.63586  -1.94285  L
H-H-0.447800          0    -7.57182   0.86112  -3.47657  L
H-H-0.447800          0    -5.46139   2.33753  -1.41928  L
H-H-0.447800          0    -4.29688   2.91133  -2.62853  L
N-N--0.415700         0    -2.17817   3.37131  -8.44972  L
C-CT--0.002400        -1   -1.30373   4.43435  -7.96421  L
C-C-0.597300          0    -1.93187   5.24312  -6.82466  L
O-O--0.567900         0    -3.03425   5.76275  -6.96209  L
C-CT--0.034300        0    -0.86876   5.31864  -9.13808  L
C-CA-0.011800         0     0.06612   4.58921  -10.08716  L
C-CA--0.125600        0     1.45315   4.5942   -9.84488  L
C-CA--0.125600        0    -0.44793   3.85415  -11.17322  L
C-CA--0.170400        0     2.32069   3.87966  -10.69065  L
C-CA--0.170400        0     0.41782   3.12442  -12.00738  L
C-CA--0.107200        0     1.80302   3.13823  -11.76782  L
H-H-0.271900          0    -2.55934   3.42923  -9.37804  L
H-H1-0.097800         0    -0.40056   3.97932  -7.56346  L
H-HC-0.029500         0    -0.3514    6.19525  -8.7444   L
H-HC-0.029500         0    -1.74877   5.67225  -9.67832  L
H-HA-0.133000         0     1.84718   5.14552  -9.00262  L
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 H-HA-0.133000        0    -1.51207   3.83806  -11.36359  L
 H-HA-0.143000        0     3.383     3.9011   -10.50769  L
 H-HA-0.143000        0     0.00975   2.55528  -12.8313   L
 H-HA-0.129700        0     2.46403   2.58115  -12.41462  L
 N-N--0.516300        0    -1.19322   5.36066  -5.71916   L
 C-CT-0.038100        0    -1.59538   6.10757  -4.52701   L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.721     7.36753  -4.40465   L
 O-O--0.581900        0     0.20868   7.43627  -3.59022   L
 C-CT--0.030300       0    -1.52278   5.19376  -3.29527   H
 C-C-0.799400         0    -2.61511   4.13723  -3.21188   H
 O-O2--0.801400       0    -2.65452   3.46774  -2.05628   H
 O-O2--0.801400       0    -3.44961   3.86731  -4.04231   H
 H-H-0.293600         0    -0.30689   4.87177  -5.70128   L
 H-H1-0.088000        0    -2.63105   6.43989  -4.63058   L
 H-HC--0.012200       0    -1.61513   5.80683  -2.39034   H
 H-HC--0.012200       0    -0.54675   4.69444  -3.25547   H
 N-N--0.516300        0    -1.02014   8.35166  -5.25513   L
 C-CT-0.038100        0    -0.25485   9.57769  -5.53359   L
 C-C-0.536600         0    -0.68978   10.79428  -4.69272  L
 O-O--0.581900        0    -0.3579    11.939    -5.00021  L
 C-CT--0.030300       0    -0.36706   9.8879    -7.03933  L
 C-C-0.799400         0    -1.74252   10.41427  -7.47044  L
 O-O2--0.801400       0    -2.74721   9.96053   -6.87533  L
 O-O2--0.801400       0    -1.77049   11.2187   -8.4282   L
 H-H-0.293600         0    -1.85      8.26299   -5.84097  L
 H-H1-0.088000        0     0.79037   9.38805   -5.31071  L
 H-HC--0.012200       0    -0.15932   8.98105   -7.60659  L
 H-HC--0.012200       0     0.39611   10.62415  -7.29905  L
 N-N--0.415700        0    -1.39205   10.54011  -3.58561  L
 C-CT--0.038900       -1   -2.10397   11.49423  -2.71056  L
 C-C-0.597300         0    -1.20395   12.64912  -2.14908  L
 O-O--0.567900        0    -1.73721   13.60225  -1.5849   L
 C-CT-0.365400        0    -2.77891   10.75447  -1.56269  L
 O-OH--0.676100       0    -1.91434   9.83761   -0.90994  L
 C-CT--0.243800       -1   -3.91926   9.97383   -2.19999  L
 H-H-0.271900         0    -1.56407   9.5612    -3.41482  L
 H-H1-0.100700        0    -2.8747    11.98848  -3.30189  L
 H-H1-0.004300        0    -3.17978   11.4598   -0.8356   L
 H-HC-0.064200        0    -4.60392   10.65648  -2.70227  L
 H-HC-0.064200        0    -4.44653   9.45817   -1.4042   L
 H-HC-0.064200        0    -3.55126   9.23268   -2.90916  L
 H-HO-0.410200        0    -1.36048   10.33996  -0.26902  L
 N-N--0.415700        0     0.13493   12.64255  -2.34103  L
 C-CT-0.014300        -1    1.07818   13.78121  -2.16144  L
 C-C-0.597300         0     2.02185   13.88602  -3.38269  L
 O-O--0.567900        0     3.14097   13.37101  -3.303    L
 C-CT--0.204100       0     1.78185   13.68286  -0.79395  L
 C-C-0.713000         0     2.8714    14.73198  -0.62181  L
 O-O--0.593100        0     2.97247   15.71736  -1.33697  L
 N-N--0.919100        0     3.76441   14.54519   0.31932  L
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H-H-0.271900          0      0.41613   11.89664  -2.96505  L
H-H1-0.104800         0      0.49244   14.69887  -2.12167  L
H-HC-0.079700         0      2.21018   12.69308  -0.66954  L
H-HC-0.079700         0      1.03785   13.82076  -0.00839  L
H-H-0.419600          0      4.42912   15.29319   0.39403  L
H-H-0.419600          0      3.66541   13.8181   1.01614  L
N-N--0.254800         0      1.63102   14.57653  -4.47941  L
C-CT--0.026600        -1     2.37008   14.60056  -5.7542   L
C-C-0.589600          0      3.75337   15.23074  -5.67544  L
O-O--0.574800         0      4.59484   15.00347  -6.54129  L
C-CT--0.007000        0      1.44905   15.28278  -6.77062  L
C-CT-0.018900         0      0.50257   16.11161  -5.90714  L
C-CT-0.019200         0      0.36089   15.27361  -4.63904  L
H-H1-0.064100         0      2.51101   13.5689  -6.07961  L
H-HC-0.025300         0      0.87559   14.52018  -7.30131  L
H-HC-0.025300         0      1.99757   15.90315  -7.4807   L
H-HC-0.021300         0     -0.45949   16.26808  -6.39623  L
H-HC-0.021300         0      0.97107   17.06617  -5.66319  L
H-H1-0.039100         0      0.14458   15.92612  -3.79317  L
H-H1-0.039100         0     -0.44103   14.54428  -4.7668   L
N-N--0.415700         0      4.04542   16.00016  -4.62925  L
C-CT--0.025200        -1     5.24751   16.82001  -4.57536  L
C-C-0.597300          0      6.53818   16.13343  -4.13117  L
O-O--0.567900         0      7.38292   16.71616  -3.4571   L
H-H-0.271900          0      3.36389   16.07029  -3.88433  L
H-H1-0.069800         0      5.0656    17.64137  -3.88228  L
H-H1-0.069800         0      5.42754   17.26015  -5.55691  L
N-N--0.347900         0      6.67918   14.8903  -4.5633   L
C-CT--0.240000        -1     7.80426   13.95722  -4.4457   L
C-C-0.734100          0      7.66882   12.8831  -5.55606  L
O-O--0.589400         0      8.39198   11.88742  -5.52144  L
C-CT--0.009400        0      7.77837   13.31647  -3.03204  L
C-CT-0.018700         0      6.36719   12.91995  -2.53771  L
C-CT--0.047900        0      6.35065   11.68559  -1.62838  L
C-CT--0.014300        0      4.96303   11.38786  -1.03013  L
N-N3--0.385400        0      3.93464   11.02206  -2.03439  L
H-H-0.274700          0      5.86699   14.59148  -5.09119  L
H-H1-0.142600         0      8.74932   14.47988  -4.59468  L
H-HC-0.036200         0      8.19373   14.03066  -2.3191   L
H-HC-0.036200         0      8.43056   12.44253  -3.02395  L
H-HC-0.010300         0      5.73865   12.70711  -3.38972  L
H-HC-0.010300         0      5.93006   13.76642  -2.00527  L
H-HC-0.062100         0      7.04633   11.8653  -0.8084   L
H-HC-0.062100         0      6.69956   10.81538  -2.18294  L
H-HP-0.113500         0      4.63176   12.27215  -0.47966  L
H-HP-0.113500         0      5.07203   10.56984  -0.31345  L
H-H-0.340000          0      3.74852   11.79189  -2.68055  L
H-H-0.340000          0      3.03339   10.81799  -1.62914  L
H-H-0.340000          0      4.18542   10.24136  -2.64118  L
N-N--0.516300         0      6.72223   13.02282  -6.50191  L
C-CT-0.039700         -1     6.2041    11.93567  -7.35719  L
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C-C-0.536600         0     6.36059   12.26767  -8.86888  L
O-O--0.581900        0     6.12343   13.39804  -9.28369  L
C-CT-0.056000        0     4.79998   11.45311  -6.95255  L
C-CT-0.013600        0     4.75344   11.30798  -5.43034  L
C-C-0.805400         0     3.90229   10.19084  -4.84463  L
O-O2--0.818800       0     2.74704   10.44744  -4.46971  L
O-O2--0.818800       0     4.51631   9.19258  -4.405    L
H-H-0.293600         0     6.20984   13.89347  -6.59399  L
H-H1-0.110500        0     6.85007   11.07291  -7.1959   L
H-HC--0.017300       0     4.62244   10.48882  -7.41998  L
H-HC--0.017300       0     4.03959   12.16069  -7.28318  L
H-HC--0.042500       0     4.43018   12.26572  -5.03715  L
H-HC--0.042500       0     5.75977   11.12378  -5.05668  L
N-N--0.415700        0     6.8413    11.3105  -9.69075  L
C-CT--0.149000      -1     7.2157    11.50223  -11.11015  L
H-H-0.271900         0     6.99909   10.40121  -9.28569  L
H-H1-0.097600        0     7.99124   12.26656  -11.18407  L
H-H1-0.097600        0     6.34227   11.84029  -11.67182  L
H-H1-0.097600        0     7.58044   10.56718  -11.53632  L
C-CT--0.366200       0     10.12176   1.88926  -12.19245  L
C-C-0.597200         0     9.02365   1.25761  -11.37178  L
O-O--0.567900        0     9.271     0.84273  -10.24409  L
H-HC-0.112300        0     10.70623   2.53503  -11.53992  L
H-HC-0.112300        0     9.70858   2.47826  -13.00827  L
H-HC-0.112300        0     10.75949   1.09853  -12.58303  L
N-N--0.415700        0     7.81279   1.20412  -11.9349  L
C-CT--0.059700      -1     6.63144   0.57852  -11.31706  L
C-C-0.597300         0     5.86482  -0.28427  -12.3371  L
O-O--0.567900        0     6.05375  -1.49599  -12.35766  L
C-CT-0.130300        0     5.74473   1.60581  -10.55266  L
C-CT--0.043000       0     6.54817   2.30504  -9.42453  L
C-CT--0.320400       0     4.50127   0.9217   -9.94295  L
C-CT--0.066000       0     5.79189   3.39149  -8.65137  L
H-H-0.271900         0     7.74036   1.55096  -12.87688  L
H-H1-0.086900        0     6.9958   -0.12836  -10.5723  L
H-HC-0.018700        0     5.40724   2.36643  -11.25865  L
H-HC-0.023600        0     7.4161    2.79825  -9.85907  L
H-HC-0.023600        0     6.90556   1.55579  -8.71598  L
H-HC-0.088200        0     3.92769   0.38495  -10.69707  L
H-HC-0.088200        0     3.83231   1.66447  -9.51138  L
H-HC-0.088200        0     4.79782   0.22236  -9.16231  L
H-HC-0.018600        0     4.97937   2.96074  -8.06696  L
H-HC-0.018600        0     5.39768   4.12913  -9.34947  L
H-HC-0.018600        0     6.4811    3.89014  -7.9689   L
N-N--0.415700        0     5.00782   0.31372  -13.17886  L
C-CT--0.149000      -1     4.16125  -0.40487  -14.13764  L
H-H-0.271900         0     4.90034   1.3116   -13.09437  L
H-H1-0.097600        0     3.70294  -1.26976  -13.65235  L
H-H1-0.097600        0     4.7675   -0.75972  -14.97292  L
H-H1-0.097600        0     3.37334   0.2491   -14.51458  L
C-CT--0.366200      -1    -4.88274   17.11272  -2.83371  L
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C-C-0.597200         0    -5.44929   16.32446  -1.66601  L
O-O--0.567900        0    -5.24398   16.72566  -0.52357  L
H-HC-0.112300        0    -5.69527   17.54207  -3.41482  L
H-HC-0.112300        0    -4.27642   16.45087  -3.45064  L
H-HC-0.112300        0    -4.25223   17.90936  -2.44299  L
N-N--0.254800        0    -6.21374   15.25163  -1.92641  L
C-CT--0.026600       -1   -6.89175   14.48491  -0.88729  L
C-C-0.589600         0    -6.02665   13.37613  -0.29161  L
O-O--0.574800        0    -5.47495   12.52416  -0.98519  L
C-CT--0.007000       0    -8.106     13.88729  -1.60802  L
C-CT-0.018900        0    -7.59312   13.63645  -3.02843  L
C-CT-0.019200        0    -6.61467   14.79055  -3.25153  L
H-H1-0.064100        0    -7.23859   15.14794  -0.09405  L
H-HC-0.025300        0    -8.90852   14.62575  -1.6385   L
H-HC-0.025300        0    -8.45855   12.97025  -1.13655  L
H-HC-0.021300        0    -8.40404   13.64937  -3.75706  L
H-HC-0.021300        0    -7.05939   12.68682  -3.07596  L
H-H1-0.039100        0    -5.75172   14.44464  -3.82277  L
H-H1-0.039100        0    -7.12085   15.59676  -3.78344  L
N-N--0.415700        0    -5.9757    13.37857   1.03276  L
C-CT--0.023700       -1   -5.12949   12.52119   1.84944  L
C-C-0.597300         0    -5.34404   10.99777   1.69246  L
O-O--0.567900        0    -6.42313   10.53528   1.3169   L
C-CT-0.034200        0    -5.37997   12.87474   3.32937  L
C-CT-0.001800        0    -4.9001    14.27603   3.73202  L
S-S--0.273700        0    -3.10524   14.46966   3.90968  L
C-CT--0.053600       -1   -2.81583   13.52541   5.43327  L
H-H-0.271900         0    -6.47212   14.12173   1.4929   L
H-H1-0.088000        0    -4.08633   12.73369   1.60582  L
H-HC-0.024100        0    -4.88653   12.14445   3.97066  L
H-HC-0.024100        0    -6.45119   12.80477   3.52613  L
H-H1-0.044000        0    -5.3578    14.53095   4.68807  L
H-H1-0.044000        0    -5.25249   15.00056   2.99773  L
H-H1-0.068400        0    -3.05268   12.47316   5.2726   L
H-H1-0.068400        0    -3.43437   13.92088   6.23845  L
H-H1-0.068400        0    -1.76487   13.60546   5.71138  L
N-N--0.415700        0    -4.31517   10.22377   2.06849  L
C-CT--0.001400       -1   -4.1793    8.77815   1.84827  L
C-C-0.597300         0    -5.40775   7.88984   2.14598  L
O-O--0.567900        0    -6.00503   7.40146   1.19379  L
C-CT--0.015200       0    -2.85891   8.24358   2.42685  L
C-CA--0.001100       0    -2.77087   6.72557   2.5072   L
C-CA--0.190600       0    -2.942     5.90886   1.36788  L
C-CA--0.190600       0    -2.65763   6.12946   3.77257  L
C-CA--0.234100       0    -3.04776   4.50663   1.5166   L
C-CA--0.234100       0    -2.78283   4.74142   3.92461  L
C-C-0.322600         0    -2.99338   3.92369   2.80192  L
O-OH--0.557900       0    -3.16916   2.58719   2.96702  L
H-H-0.271900         0    -3.48174   10.70131   2.37999  L
H-H1-0.087600        0    -4.05683   8.67759   0.76943  L
H-HC-0.029500        0    -2.73719   8.65584   3.4263   L
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H-HC-0.029500        0    -2.03198   8.6126    1.81896  L
H-HA-0.169900        0    -3.08441   6.37091   0.3981   L
H-HA-0.169900        0    -2.56266   6.74507   4.65344  L
H-HA-0.165600        0    -3.26435   3.86938   0.66999  L
H-HA-0.165600        0    -2.7943    4.32155   4.91763  L
H-HO-0.399200        0    -3.48114   2.4146    3.8759   L
N-N--0.516300        0    -5.76825   7.59567   3.40006  L
C-CT-0.038100        -1   -6.74651   6.53931   3.76097  L
C-C-0.536600         0    -8.15152   6.79197   3.21166  L
O-O--0.581900        0    -8.83253   5.84846   2.81832  L
C-CT--0.030300       0    -6.77277   6.34699   5.28861  L
C-C-0.799400         0    -5.48059   5.70933   5.81795  L
O-O2--0.801400       0    -5.35467   4.46492   5.71199  L
O-O2--0.801400       0    -4.60268   6.4661    6.30525  L
H-H-0.293600         0    -5.25725   8.05847   4.14646  L
H-H1-0.088000        0    -6.40165   5.59811   3.33646  L
H-HC--0.012200       0    -7.60645   5.69288   5.54685  L
H-HC--0.012200       0    -6.94452   7.30837   5.7761   L
N-N--0.415700        0    -8.56773   8.0589    3.1407   L
C-CT--0.002400       0    -9.757     8.48721   2.40237  L
C-C-0.597300         0    -9.67899   8.05728   0.92898  L
O-O--0.567900        0    -10.54654   7.33434   0.43966  L
C-CT--0.034300       0    -9.92473   10.00801   2.54297  L
C-CA-0.011800        0    -10.98131   10.58969   1.62219  L
C-CA--0.125600       0    -12.3468   10.45911   1.93738  L
C-CA--0.125600       0    -10.59913   11.20849   0.41611  L
C-CA--0.170400       0    -13.3246   10.94962   1.05282  L
C-CA--0.170400       0    -11.57607   11.69628  -0.46911  L
C-CA--0.107200       0    -12.93943   11.56765  -0.15042  L
H-H-0.271900         0    -7.90297   8.75371   3.44737  L
H-H1-0.097800        0    -10.63351   7.99992   2.83126  L
H-HC-0.029500        0    -8.97189   10.49497   2.32971  L
H-HC-0.029500        0    -10.18662   10.2399   3.57606  L
H-HA-0.133000        0    -12.64628   9.96354   2.84979  L
H-HA-0.133000        0    -9.5525    11.28277   0.1525   L
H-HA-0.143000        0    -14.37241   10.8351   1.29044  L
H-HA-0.143000        0    -11.27451   12.15068  -1.4023   L
H-HA-0.129700        0    -13.69062   11.93026  -0.8375   L
N-N--0.415700        0    -8.64283   8.49182   0.21357  L
C-CT--0.038900       -1   -8.47253   8.19931  -1.21406  L
C-C-0.597300         0    -8.33174   6.71852  -1.51315  L
O-O--0.567900        0    -8.9997    6.18686  -2.39734  L
C-CT-0.365400        0    -7.30471   9.00682  -1.79198  L
O-OH--0.676100       0    -7.52547   10.37974  -1.54438  L
C-CT--0.243800       0    -7.1714    8.84829  -3.30703  L
H-H-0.271900         0    -7.95349   9.09136   0.6561   L
H-H1-0.100700        0    -9.37365   8.53459  -1.72731  L
H-H1-0.004300        0    -6.38793   8.68829  -1.30192  L
H-HC-0.064200        0    -8.11657   9.09686  -3.79001  L
H-HC-0.064200        0    -6.89493   7.82435  -3.5575   L
H-HC-0.064200        0    -6.39917   9.516    -3.68639  L
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H-HO-0.410200        0    -6.66985   10.80157  -1.37295  L
N-N--0.415700        0    -7.49048   6.04859  -0.73574  L
C-CT--0.058100       -1   -7.36268   4.6034   -0.65079  L
C-C-0.597300         0    -8.71552   3.9213   -0.50851  L
O-O--0.567900        0    -9.03915   3.07228  -1.33795  L
C-CT--0.007400       0    -6.39712   4.29751   0.4933   L
C-CC-0.186800        0    -6.34885   2.85995   0.90935  L
N-NB--0.543200       0    -6.52316   1.76762   0.0646   L
C-CW--0.220700       0    -6.23461   2.42749   2.19265  L
C-CR-0.163500        0    -6.53821   0.68904   0.8557   L
N-NA--0.279500       0    -6.3515    1.06071   2.13216  L
H-H-0.271900         0    -7.00422   6.60193  -0.03753  L
H-H1-0.136000        0    -6.93267   4.24162  -1.58292  L
H-HC-0.036700        0    -6.70063   4.87381   1.3617   L
H-HC-0.036700        0    -5.40206   4.62043   0.19707  L
H-H4-0.186200        0    -6.12211   3.04137   3.07829  L
H-H-0.333900         0    -6.35615   0.42438   2.9262   L
H-H5-0.143500        0    -6.70303  -0.32576   0.5158   L
N-N--0.415700        0    -9.5091    4.29582   0.49996  L
C-CT-0.021300        -1   -10.81362   3.68165   0.69876  L
C-C-0.597300         0    -11.72941   3.76016  -0.50046  L
O-O--0.567900        0    -12.35475   2.77201  -0.88138  L
C-CT--0.123100       0    -11.46045   4.05917   2.04872  L
S-SH--0.311900       0    -12.5195   5.53324   2.00336  L
H-H-0.271900         0    -9.19638   5.00483   1.15536  L
H-H1-0.112400        0    -10.60541   2.61385   0.78481  L
H-H1-0.111200        0    -10.68454   4.19442   2.80167  L
H-H1-0.111200        0    -12.07863   3.21998   2.3718   L
H-HS-0.193300        0    -11.59503   6.36585   1.50575  L
N-N--0.415700        0    -11.7585   4.93329  -1.11079  L
C-CT--0.059700       -1   -12.58325   5.18571  -2.2646   L
C-C-0.597300         0    -12.12917   4.47158  -3.53877  L
O-O--0.567900        0    -12.95671   3.87053  -4.2199   L
C-CT-0.130300        0    -12.79209   6.71655  -2.41853  L
C-CT--0.043000       0    -14.11796   7.16955  -1.75714  L
C-CT--0.320400       -1   -12.70171   7.2447   -3.8546   L
C-CT--0.066000       -1   -15.41758   6.79512  -2.50097  L
H-H-0.271900         0    -11.20592   5.68348  -0.71013  L
H-H1-0.086900        0    -13.55837   4.75004  -2.04883  L
H-HC-0.018700        0    -11.98875   7.22045  -1.87719  L
H-HC-0.023600        0    -14.09407   8.25509  -1.65177  L
H-HC-0.023600        0    -14.16246   6.75134  -0.75028  L
H-HC-0.088200        0    -11.6874   7.12002  -4.23529  L
H-HC-0.088200        0    -12.93532   8.30929  -3.87073  L
H-HC-0.088200        0    -13.39777   6.71554  -4.50709  L
H-HC-0.018600        0    -16.27444   7.10484  -1.90244  L
H-HC-0.018600        0    -15.47045   5.71799  -2.65887  L
H-HC-0.018600        0    -15.46419   7.30473  -3.46318  L
N-N--0.415700        0    -10.84171   4.53994  -3.87233  L
C-CT--0.024900       -1   -10.25593   3.85176  -5.02826  L
C-C-0.597300         0    -10.48117   2.32888  -4.89506  L
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O-O--0.567900        0    -10.9421   1.70522  -5.84381  L
C-CT-0.211700        0    -8.79032   4.28175  -5.13929  L
O-OH--0.654600       0    -8.33605   4.19402  -6.47324  L
H-H-0.271900         0    -10.23215   5.06436  -3.25303  L
H-H1-0.084300        0    -10.77693   4.18461  -5.92648  L
H-H1-0.035200        0    -8.17026   3.68556  -4.47022  L
H-H1-0.035200        0    -8.70757   5.32747  -4.84007  L
H-HO-0.427500        0    -7.53179   4.71535  -6.56104  L
N-N--0.516300        0    -10.27509   1.73048  -3.70701  L
C-CT-0.038100        -1   -10.60609   0.31344  -3.43441  L
C-C-0.536600         0    -12.0942  -0.03908  -3.58509  L
O-O--0.581900        0    -12.44265  -0.97149  -4.31505  L
C-CT--0.030300       0    -10.10598  -0.1486   -2.04442  L
C-C-0.799400         0    -8.75078  -0.85051  -2.10474  L
O-O2--0.801400       0    -8.13596  -0.86721  -3.18999  L
O-O2--0.801400       0    -8.26323  -1.35585  -1.07034  L
H-H-0.293600         0    -9.93556   2.29975  -2.93881  L
H-H1-0.088000        0    -10.11978  -0.27599  -4.20764  L
H-HC--0.012200       0    -10.81695  -0.86109  -1.62295  L
H-HC--0.012200       0    -10.05766   0.69712  -1.35923  L
N-N--0.415700        0    -12.96774   0.67898  -2.8745   L
C-CT-0.033700        -1   -14.42333   0.55573  -2.96385  L
C-C-0.597300         0    -14.91855   0.60101  -4.42201  L
O-O--0.567900        0    -15.76996  -0.19272  -4.81829  L
C-CT--0.182500       -1   -15.01508   1.71231  -2.21636  L
H-H-0.271900         0    -12.59849   1.41774  -2.28462  L
H-H1-0.082300        0    -14.74453  -0.38567  -2.51736  L
H-HC-0.060300        0    -14.73479   1.65259  -1.16432  L
H-HC-0.060300        0    -16.10313   1.67105  -2.2834   L
H-HC-0.060300        0    -14.67031   2.6613   -2.62577  L
N-N--0.415700        0    -14.41306   1.57396  -5.18726  L
C-CT--0.025200       -1   -14.78029   1.85561  -6.56993  L
C-C-0.597300         0    -14.30769   0.80306  -7.5689   L
O-O--0.567900        0    -15.05977   0.41915  -8.45975  L
H-H-0.271900         0    -13.73151   2.18942  -4.75465  L
H-H1-0.069800        0    -14.35167   2.81355  -6.86187  L
H-H1-0.069800        0    -15.86537   1.9258   -6.64298  L
N-N--0.516300        0    -13.05967   0.36177  -7.42934  L
C-CT-0.039700        -1   -12.44688  -0.72744  -8.1941   L
C-C-0.536600         0    -13.20047  -2.06207  -8.04011  L
O-O--0.581900        0    -13.3582   -2.8005   -9.00936  L
C-CT-0.056000        0    -10.9817   -0.82168  -7.73373  L
C-CT-0.013600        0    -10.12313  -1.91216  -8.38245  L
C-C-0.805400         0    -9.64376   -1.5903   -9.7987   L
O-O2--0.818800       0    -9.68133   -2.49704  -10.66054  L
O-O2--0.818800       0    -9.07019   -0.49796  -9.99964  L
H-H-0.293600         0    -12.48279   0.7888   -6.71022  L
H-H1-0.110500        0    -12.45933  -0.4726   -9.25457  L
H-HC--0.017300       0    -10.98959  -1.00548  -6.66106  L
H-HC--0.017300       0    -10.49637   0.14114  -7.89358  L
H-HC--0.042500       0    -10.67474  -2.8477   -8.36645  L
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H-HC--0.042500       0    -9.23119  -2.04735  -7.7687   L
N-N--0.415700        0    -13.64956  -2.38211  -6.82157  L
C-CT--0.025200       -1   -14.36725  -3.62225  -6.48811  L
C-C-0.597300         0    -13.63029  -4.50408  -5.49573  L
O-O--0.567900        0    -13.98824  -5.67554  -5.35163  L
H-H-0.271900         0    -13.50698  -1.68404  -6.1002   L
H-H1-0.069800        0    -14.54723  -4.20818  -7.38985  L
H-H1-0.069800        0    -15.33243  -3.36119  -6.05594  L
N-N--0.415700        0    -12.60934  -3.96857  -4.80959  L
C-CT--0.059700       -1   -11.87789  -4.70654  -3.77902  L
C-C-0.597300         0    -12.89522  -5.24404  -2.76795  L
O-O--0.567900        0    -13.80723  -4.53422  -2.34964  L
C-CT-0.130300        0    -10.77126  -3.85253  -3.10885  L
C-CT--0.043000       0    -9.47991  -3.88618  -3.94153  L
C-CT--0.320400       0    -10.35685  -4.37339  -1.71559  L
C-CT--0.066000       0    -9.53409  -3.18951  -5.29514  L
H-H-0.271900         0    -12.43635  -2.97583  -4.92644  L
H-H1-0.086900        0    -11.41509  -5.55801  -4.261    L
H-HC-0.018700        0    -11.11576  -2.8261   -2.99549  L
H-HC-0.023600        0    -9.23088  -4.92222  -4.11239  L
H-HC-0.023600        0    -8.67165  -3.4382   -3.36808  L
H-HC-0.088200        0    -9.56521  -3.74469  -1.30498  L
H-HC-0.088200        0    -9.99805  -5.401    -1.78395  L
H-HC-0.088200        0    -11.194   -4.31976  -1.02683  L
H-HC-0.018600        0    -8.55585  -3.25041  -5.76952  L
H-HC-0.018600        0    -9.79218  -2.14536  -5.15525  L
H-HC-0.018600        0    -10.26577  -3.66772  -5.94186  L
N-N--0.415700        0    -12.73283  -6.50835  -2.37463  L
C-CT--0.025200       -1   -13.59227  -7.16072  -1.37886  L
C-C-0.597300         0    -13.03231  -7.12723   0.02632  L
O-O--0.567900        0    -13.75282  -6.93161   1.00303  L
H-H-0.271900         0    -12.00308  -7.01927  -2.85488  L
H-H1-0.069800        0    -13.73748  -8.20176  -1.66299  L
H-H1-0.069800        0    -14.57262  -6.68183  -1.36574  L
N-N--0.415700        0    -11.72596  -7.338     0.1099   L
C-CT--0.058100       -1   -10.96786  -7.36029   1.34229  L
C-C-0.597300         0    -9.58081  -6.73511   1.0811   L
O-O--0.567900        0    -8.85121  -7.22206   0.21829  L
C-CT--0.007400       0    -10.84035  -8.81404   1.83012  L
C-CC-0.186800        0    -12.14417  -9.38944   2.33513  L
N-NB--0.543200       0    -12.73548  -9.11755   3.57218  L
C-CW--0.220700       0    -12.97499  -10.19802   1.61604  L
C-CR-0.163500        0    -13.9149  -9.75392   3.5629   L
N-NA--0.279500       0    -14.08471  -10.4154   2.40425  L
H-H-0.271900         0    -11.21055  -7.44819  -0.75165  L
H-H1-0.136000        0    -11.47617  -6.77646   2.11129  L
H-HC-0.036700        0    -10.10107  -8.86397   2.62707  L
H-HC-0.036700        0    -10.46947  -9.436     1.01397  L
H-H4-0.186200        0    -12.7991  -10.54781   0.60895  L
H-H-0.333900         0    -14.91023  -10.93706   2.1495   L
H-H5-0.143500        0    -14.63171  -9.72527   4.37349  L
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N-N--0.415700        0    -9.21479  -5.64564   1.7688   L
C-CT--0.024900       -1   -7.94613  -4.92477   1.54127  L
C-C-0.597300         0    -6.75761  -5.57967   2.24721  L
O-O--0.567900        0    -6.79045  -5.85413   3.44641  L
C-CT-0.211700        0    -8.05467  -3.4359    1.89108  L
O-OH--0.654600       0    -6.76857  -2.82897   1.85854  L
H-H-0.271900         0    -9.82589  -5.34896   2.52176  L
H-H1-0.084300        0    -7.74125  -4.95905   0.47052  L
H-H1-0.035200        0    -8.4896   -3.32912   2.87794  L
H-H1-0.035200        0    -8.71015  -2.94058   1.17235  L
H-HO-0.427500        0    -6.77086  -2.07524   2.47829  L
N-N--0.415700        0    -5.67691  -5.79629   1.49469  L
C-CT--0.051800       -1   -4.37534  -6.2099    2.01535  L
C-C-0.597300         0    -3.48742  -5.00387   2.26327  L
O-O--0.567900        0    -3.2798   -4.20211   1.35503  L
C-CT--0.110200       0    -3.69448  -7.18243   1.02893  L
C-CT-0.353100        0    -4.22737  -8.62853   1.01498  L
C-CT--0.412100       0    -5.59856  -8.77293   0.3538   L
C-CT--0.412100       0    -3.24841  -9.51158   0.23418  L
H-H-0.271900         0    -5.76287  -5.58983   0.51118  L
H-H1-0.092200        0    -4.51363  -6.72923   2.96689  L
H-HC-0.045700        0    -2.64384  -7.2347    1.305    L
H-HC-0.045700        0    -3.74004  -6.7731    0.02314  L
H-HC--0.036100       0    -4.28216  -9.00069   2.03828  L
H-HC-0.100000        0    -5.58444  -8.34462  -0.64906  L
H-HC-0.100000        0    -6.35972  -8.27187   0.94933  L
H-HC-0.100000        0    -5.87266  -9.8248    0.29081  L
H-HC-0.100000        0    -2.26253  -9.47111   0.6966   L
H-HC-0.100000        0    -3.18048  -9.16737  -0.79832  L
H-HC-0.100000        0    -3.59774  -10.54392   0.24281  L
N-N--0.415700        0    -2.92342  -4.91547   3.46054  L
C-CT-0.021300        -1   -1.96473  -3.87637   3.8066   L
C-C-0.597300         0    -0.83422  -4.42284   4.69648  L
O-O--0.567900        0    -0.85024  -5.59066   5.08809  L
C-CT--0.123100       0    -2.75263  -2.73485   4.45855  L
S-SH--0.311900       0    -1.7875   -1.20266   4.48621  L
H-H-0.271900         0    -3.17394  -5.59214   4.17351  L
H-H1-0.112400        0    -1.49879  -3.4901    2.89649  L
H-H1-0.111200        0    -3.04661  -3.01262   5.47229  L
H-H1-0.111200        0    -3.65227  -2.54937   3.87079  L
H-HS-0.193300        0    -2.68575  -0.48461   5.17475  L
N-N--0.415700        0     0.16099  -3.60469   5.0362   L
C-CT--0.038900       -1    1.27684  -4.00535   5.90602  L
C-C-0.597300         0     1.40336  -3.14703   7.14055  L
O-O--0.567900        0     0.72834  -2.14141   7.33727  L
C-CT-0.365400        0     2.62427  -4.0886    5.16177  L
O-OH--0.676100       0     2.99707  -2.87      4.55295  L
C-CT--0.243800       0     2.6205   -5.20305   4.11941  L
H-H-0.271900         0     0.08007  -2.63873   4.74137  L
H-H1-0.100700        0     1.07625  -5.00868   6.28207  L
H-H1-0.004300        0     3.40586  -4.34696   5.87625  L
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H-HC-0.064200        0     1.89717  -4.99405   3.33299  L
H-HC-0.064200        0     2.35549  -6.14932   4.59234  L
H-HC-0.064200        0     3.61243  -5.28996   3.68659  L
H-HO-0.410200        0     3.37294  -2.28714   5.25023  L
N-N--0.415700        0     2.25897  -3.6413    8.02431  L
C-CT--0.051800       -1    2.18358  -3.3607    9.43465  L
C-C-0.597300         0     2.28821  -1.86788   9.83194  L
O-O--0.567900        0     1.73348  -1.48386   10.85226  L
C-CT--0.110200       0     3.18401  -4.25006   10.14081  L
C-CT-0.353100        0     2.88819  -4.34915   11.63882  L
C-CT--0.412100       0     1.54178  -4.9888    11.98936  L
C-CT--0.412100       -1    3.97398  -5.26461   12.1405  L
H-H-0.271900         0     2.72016  -4.49235   7.75651  L
H-H1-0.092200        0     1.18021  -3.66291   9.73625  L
H-HC-0.045700        0     4.184    -3.84294   9.98261  L
H-HC-0.045700        0     3.13458  -5.25167   9.70858  L
H-HC--0.036100       0     2.98877  -3.38119   12.12669  L
H-HC-0.100000        0     1.41016  -5.93397   11.46388  L
H-HC-0.100000        0     0.72703  -4.31511   11.73165  L
H-HC-0.100000        0     1.48203  -5.15919   13.06533  L
H-HC-0.100000        0     3.87007  -5.37274   13.221   L
H-HC-0.100000        0     4.95536  -4.8356    11.94093  L
H-HC-0.100000        0     3.89288  -6.25136   11.68459  L
N-N--0.516300        0     2.96519  -1.01852   9.05344  L
C-CT-0.039700        -1    3.11448   0.42854   9.3254   L
C-C-0.536600         0     1.88297   1.29996   8.98319  L
O-O--0.581900        0     1.98494   2.5273    8.92099  L
C-CT-0.056000        0     4.39693   0.92432   8.61913  L
C-CT-0.013600        0     4.40963   0.87251   7.07737  L
C-C-0.805400         0     4.96132  -0.4298    6.48336  L
O-O2--0.818800       0     4.28233  -1.48538   6.51189  L
O-O2--0.818800       0     6.12431  -0.43206   6.0013   L
H-H-0.293600         0     3.30236  -1.37189   8.16229  L
H-H1-0.110500        0     3.26376   0.55992   10.39828  L
H-HC--0.017300       0     5.25099   0.35798   8.99478  L
H-HC--0.017300       0     4.55967   1.9607    8.91788  L
H-HC--0.042500       0     5.06852   1.67484   6.74304  L
H-HC--0.042500       0     3.41317   1.07037   6.6849   L
N-N--0.415700        0     0.72081   0.67036   8.79812  L
C-CT--0.002400       -1   -0.58774   1.30304   8.59312  L
C-C-0.597300         0    -1.72469   0.67512   9.41446  L
O-O--0.567900        0    -2.89681   1.01622   9.24633  L
C-CT--0.034300       0    -0.97518   1.1286    7.11148  L
C-CA-0.011800        0    -0.04889   1.64451   6.02209  L
C-CA--0.125600       0    -0.26189   2.92366   5.48062  L
C-CA--0.125600       0     0.90078   0.79252   5.42449  L
C-CA--0.170400       0     0.42646   3.32857   4.32448  L
C-CA--0.170400       0     1.62027   1.20935   4.28984  L
C-CA--0.107200       0     1.37263   2.47399   3.73125  L
H-H-0.271900         0     0.7608   -0.3394    8.76073  L
H-H1-0.097800        0    -0.53355   2.36508   8.83128  L
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H-HC-0.029500        0    -1.94313   1.60452   6.95594  L
H-HC-0.029500        0    -1.12752   0.06264   6.94081  L
H-HA-0.133000        0    -0.98874   3.58137   5.93338  L
H-HA-0.133000        0     1.05252  -0.20012   5.81709  L
H-HA-0.143000        0     0.21429   4.30108   3.90488  L
H-HA-0.143000        0     2.33922   0.54613   3.8298   L
H-HA-0.129700        0     1.91616   2.78317   2.85045  L
N-N--0.415700        0    -1.37151  -0.26265   10.28255  L
C-CT--0.003100      -1    -2.24281  -1.14553   11.04018  L
C-C-0.597300         0    -3.47806  -0.44708   11.66692  L
O-O--0.567900        0    -4.62279  -0.77311   11.36984  L
C-CT--0.003600       0    -1.32529  -1.76483   12.11528  L
C-CT--0.064500       0    -1.98413  -2.51907   13.2831  L
C-C-0.695100         0    -1.04662  -2.58501   14.48771  L
O-O--0.608600        0    -0.59341  -3.64158   14.89719  L
N-N--0.940700        0    -0.71612  -1.47275   15.11376  L
H-H-0.271900         0    -0.37538  -0.36659   10.42922  L
H-H1-0.085000        0    -2.6252   -1.93064   10.40086  L
H-HC-0.017100        0    -0.73108  -0.95355   12.53948  L
H-HC-0.017100        0    -0.62931  -2.4429    11.6235  L
H-HC-0.035200        0    -2.24116  -3.52826   12.96022  L
H-HC-0.035200        0    -2.89621  -2.02707   13.61326  L
H-H-0.425100         0    -0.08142  -1.60731   15.87422  L
H-H-0.425100         0    -0.97867  -0.534     14.80197  L
N-N--0.516300        0    -3.24742   0.45711   12.61272  L
C-CT-0.038100       -1    -4.20411   1.33054   13.32892  L
C-C-0.536600         0    -4.76895   2.42475   12.41993  L
O-O--0.581900        0    -5.95571   2.74237   12.49202  L
C-CT--0.030300       0    -3.45988   1.94331   14.5339  L
C-C-0.799400         0    -1.99524   2.23439   14.18569  L
O-O2--0.801400       0    -1.73392   3.24643   13.49827  L
O-O2--0.801400       0    -1.16647   1.31048   14.38264  L
H-H-0.293600         0    -2.26571   0.59479   12.82881  L
H-H1-0.088000        0    -5.04586   0.74063   13.69265  L
H-HC--0.012200       0    -3.48747   1.22786   15.35781  L
H-HC--0.012200       0    -3.96088   2.85559   14.86212  L
N-N--0.415700        0    -3.92131   2.9751    11.54612  L
C-CT-0.014300       -1    -4.26737   4.01086   10.57675  L
C-C-0.597300         0    -5.52037   3.6979    9.75958  L
O-O--0.567900        0    -6.29654   4.59723   9.43645  L
C-CT--0.204100       0    -3.0641    4.33523   9.67029  L
C-C-0.713000         0    -2.07086   5.32764   10.24801  L
O-O--0.593100        0    -1.66487   6.26255   9.57763  L
N-N--0.919100        0    -1.60016   5.17695   11.46454  L
H-H-0.271900         0    -2.96545   2.6549    11.60269  L
H-H1-0.104800        0    -4.51552   4.91702   11.13271  L
H-HC-0.079700        0    -3.44441   4.77852   8.74768  L
H-HC-0.079700        0    -2.53114   3.43434   9.39608  L
H-H-0.419600         0    -0.95673   5.89449   11.73335  L
H-H-0.419600         0    -1.85571   4.43672   12.12202  L
N-N--0.347900        0    -5.73408   2.4159    9.4591   L
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C-CT--0.263700       -1   -6.88909   1.94101   8.70598  L
C-C-0.734100         0    -8.2781    2.26422   9.27321  L
O-O--0.589400        0    -9.26975   2.09223   8.56745  L
C-CT--0.000700       0    -6.73226   0.44224   8.39219  L
C-CT-0.039000        0    -7.32729  -0.45535   9.48134  L
C-CT-0.048600        0    -6.94156  -1.91872   9.2837   L
N-N2--0.529500       0    -7.61748  -2.73023   10.30195  L
C-CA-0.807600        0    -7.10341  -3.13904   11.4361  L
N-N2--0.862700       0    -5.83067  -3.25583   11.64693  L
N-N2--0.862700       0    -7.88496  -3.38545   12.43814  L
H-H-0.274700         0    -5.01323   1.76092   9.74309  L
H-H1-0.156000        0    -6.85548   2.46429   7.7484   L
H-HC-0.032700        0    -5.67353   0.2082    8.26553  L
H-HC-0.032700        0    -7.2445    0.22507   7.4533   L
H-HC-0.028500        0    -8.41533  -0.38025   9.45983  L
H-HC-0.028500        0    -6.97545  -0.12278   10.45832  L
H-H1-0.068700        0    -5.86003  -2.00177   9.36297  L
H-H1-0.068700        0    -7.242    -2.25613   8.29511  L
H-H-0.345600         0    -8.62767  -2.77622   10.26011  L
H-H-0.447800         0    -5.44652  -2.3257    11.76888  L
H-H-0.447800         0    -5.36401  -3.59379   10.79562  L
H-H-0.447800         0    -7.45469  -3.65157   13.2983  L
H-H-0.447800         0    -8.8565   -3.08993   12.35074  L
N-N--0.415700        0    -8.38532   2.70492   10.52328  L
C-CT--0.149000       -1   -9.66446   3.05254   11.11723  L
H-H-0.271900         0    -7.52897   2.81026   11.05653  L
H-H1-0.097600        0    -10.23973   3.6824    10.43757  L
H-H1-0.097600        0    -9.50022   3.58845   12.05269  L
H-H1-0.097600        0    -10.22685   2.13932   11.32252  L
C-CT--0.366200       -1   -9.84132   6.2993    8.97399  L
C-C-0.597200         0    -10.57086   5.58625   7.85948  L
O-O--0.567900        0    -11.74782   5.85617   7.6609   L
H-HC-0.112300        0    -9.02676   5.67943   9.34929  L
H-HC-0.112300        0    -10.54186   6.51236   9.77853  L
H-HC-0.112300        0    -9.43706   7.23152   8.58429  L
N-N--0.415700        0    -9.89615   4.66973   7.1619   L
C-CT--0.001400       -1   -10.43698   3.84965   6.05784  L
C-C-0.597300         0    -11.77766   3.16339   6.35745  L
O-O--0.567900        0    -12.65868   3.0521    5.50226  L
C-CT--0.015200       0    -9.31551   2.94683   5.49131  L
C-CA--0.001100       0    -9.7262    1.72471   4.68972  L
C-CA--0.190600       0    -10.34969   0.64153   5.3386   L
C-CA--0.190600       0    -9.4195    1.63466   3.31685  L
C-CA--0.234100       0    -10.72005  -0.49949   4.60787  L
C-CA--0.234100       0    -9.7469    0.47274   2.58997  L
C-C-0.322600         0    -10.40784  -0.58998   3.23681  L
O-OH--0.557900       0    -10.75722  -1.70456   2.5522   L
H-H-0.271900         0    -8.93221   4.52022   7.41952  L
H-H1-0.087600        0    -10.68004   4.54569   5.25331  L
H-HC-0.029500        0    -8.67791   2.595     6.2947   L
H-HC-0.029500        0    -8.67556   3.57259   4.86776  L
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H-HA-0.169900        0    -10.55394   0.69335   6.39867  L
H-HA-0.169900        0    -8.91776   2.45282   2.81865  L
H-HA-0.165600        0    -11.22974  -1.31463   5.09223  L
H-HA-0.165600        0    -9.5116    0.38527   1.53765  L
H-HO-0.399200        0    -11.67072  -1.92045   2.80999  L
N-N--0.516300        0    -11.9459   2.72719   7.59819  L
C-CT-0.038100        -1   -13.17783   2.16644   8.12999  L
C-C-0.536600         0    -14.36776   3.1383    8.3115   L
O-O--0.581900        0    -15.50876   2.65783   8.35785  L
C-CT--0.030300       0    -12.85098   1.56958   9.52293  L
C-C-0.799400         0    -12.16529   0.19865   9.48709  L
O-O2--0.801400       0    -12.70288  -0.70457   8.80718  L
O-O2--0.801400       0    -11.15442  -0.02708   10.18297  L
H-H-0.293600         0    -11.11328   2.75493   8.17915  L
H-H1-0.088000        0    -13.51189   1.36688   7.46841  L
H-HC--0.012200       0    -13.77929   1.44232   10.08179  L
H-HC--0.012200       0    -12.24262   2.27788   10.08606  L
N-N--0.415700        0    -14.11076   4.44226   8.51449  L
C-CT--0.149000       -1   -15.04584   5.48922   8.954    L
H-H-0.271900         0    -13.15467   4.73394   8.32772  L
H-H1-0.097600        0    -15.95375   5.44451   8.35031  L
H-H1-0.097600        0    -14.58024   6.46823   8.82818  L
H-H1-0.097600        0    -15.30297   5.33887   10.00288  L
C-CT--0.366200       -1   -19.83337  -0.85349  -1.23148  L
C-C-0.597200         0    -18.82484  -0.52908  -0.11812  L
O-O--0.567900        0    -18.42309   0.62361  -0.02278  L
H-HC-0.112300        0    -20.69185  -1.36977  -0.80904  L
H-HC-0.112300        0    -19.34385  -1.4748   -1.98006  L
H-HC-0.112300        0    -20.15438   0.07755  -1.69686  L
N-N--0.415700        0    -18.40327  -1.49206   0.73161  L
C-CT--0.058100       -1   -17.27282  -1.29879   1.6895   L
C-C-0.597300         0    -16.43965  -2.54519   2.00334  L
O-O--0.567900        0    -16.86971  -3.37277   2.8117   L
C-CT--0.007400       0    -17.70151  -0.53898   2.95572  L
C-CC-0.186800        0    -16.51041   0.17964   3.54582  L
N-NB--0.543200       0    -15.47321  -0.4447    4.22947  L
C-CW--0.220700       0    -16.17145   1.48703   3.34237  L
C-CR-0.163500        0    -14.50668   0.47767   4.38245  L
N-NA--0.279500       0    -14.91901   1.66092   3.90321  L
H-H-0.271900         0    -18.77022  -2.42249   0.6106   L
H-H1-0.136000        0    -16.60957  -0.59431   1.19324  L
H-HC-0.036700        0    -18.12562  -1.22598   3.68837  L
H-HC-0.036700        0    -18.45721   0.20494   2.70168  L
H-H4-0.186200        0    -16.7401   2.21115   2.77291  L
H-H-0.333900         0    -14.34223   2.49993   3.93134  L
H-H5-0.143500        0    -13.53778   0.30353   4.83684  L
N-N--0.254800        0    -15.24145  -2.68134   1.40479  L
C-CT--0.026600       -1   -14.2974  -3.7132    1.79888  L
C-C-0.589600         0    -13.60841  -3.41121   3.12006  L
O-O--0.574800        0    -13.21744  -2.27433   3.3858   L
C-CT--0.007000       0    -13.24545  -3.74693   0.6982   L
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C-CT-0.018900        0    -13.2642  -2.34634   0.0886   L
C-CT-0.019200        0    -14.7058  -1.89273   0.29388  L
H-H1-0.064100        0    -14.79702  -4.68094   1.85864  L
H-HC-0.025300        0    -13.57063  -4.47408  -0.02936  L
H-HC-0.025300        0    -12.2555  -4.01382   1.07168  L
H-HC-0.021300        0    -12.99045  -2.35463  -0.96681  L
H-HC-0.021300        0    -12.59733  -1.68815   0.64378  L
H-H1-0.039100        0    -14.70681  -0.82466   0.5126   L
H-H1-0.039100        0    -15.2843  -2.09594  -0.60882  L
N-N--0.347900        0    -13.3352  -4.44745   3.91478  L
C-CT--0.263700       -1   -12.56644  -4.29552   5.15698  L
C-C-0.734100         0    -11.06179  -4.65491   4.97288  L
O-O--0.589400        0    -10.7507  -5.49863   4.13795  L
C-CT--0.000700       0    -13.29646  -4.95217   6.34156  L
C-CT-0.039000        0    -14.6042  -4.19209   6.6811   L
C-CT-0.048600        0    -14.37113  -2.82157   7.35478  L
N-N2--0.529500       0    -15.27984  -1.7607    6.86005  L
C-CA-0.807600        0    -15.67565  -0.66879   7.5002   L
N-N2--0.862700       0    -15.37818  -0.42337   8.73589  L
N-N2--0.862700       0    -16.34461   0.26749   6.89897  L
H-H-0.274700         0    -13.60046  -5.36807   3.58811  L
H-H1-0.156000        0    -12.52665  -3.23415   5.39254  L
H-HC-0.032700        0    -12.64699  -4.95665   7.21889  L
H-HC-0.032700        0    -13.53477  -5.98524   6.08526  L
H-HC-0.028500        0    -15.19676  -4.80558   7.36042  L
H-HC-0.028500        0    -15.19175  -4.05999   5.77135  L
H-H1-0.068700        0    -13.3488  -2.49693   7.16709  L
H-H1-0.068700        0    -14.47891  -2.94291   8.43413  L
H-H-0.345600         0    -15.47821  -1.7512    5.86453  L
H-H-0.447800         0    -15.59505   0.496     9.07846  L
H-H-0.447800         0    -14.49287  -0.85728   8.99915  L
H-H-0.447800         0    -16.40934   1.17478   7.34451  L
H-H-0.447800         0    -16.39042   0.19678   5.88917  L
N-N--0.415700        0    -10.12441  -3.96566   5.65491  L
C-CT--0.003100       -1   -8.64003  -4.08481   5.52675  L
C-C-0.597300         0    -8.04494  -4.94237   6.65061  L
O-O--0.567900        0    -8.49188  -4.87286   7.79731  L
C-CT--0.003600       0    -7.99589  -2.69125   5.50274  L
C-CT--0.064500       0    -6.4624   -2.77829   5.40641  L
C-C-0.695100         0    -5.86106  -1.45658   4.98046  L
O-O--0.608600        0    -6.10841  -1.0101    3.87318  L
N-N--0.940700        0    -5.04552  -0.81717   5.78437  L
H-H-0.271900         0    -10.45837  -3.28814   6.33068  L
H-H1-0.085000        0    -8.42691  -4.58255   4.58689  L
H-HC-0.017100        0    -8.27117  -2.13669   6.39816  L
H-HC-0.017100        0    -8.38297  -2.14112   4.6473   L
H-HC-0.035200        0    -6.18152  -3.5183    4.65799  L
H-HC-0.035200        0    -6.05085  -3.082     6.36651  L
H-H-0.425100         0    -4.75558   0.11623   5.52197  L
H-H-0.425100         0    -4.71546  -1.29231   6.63547  L
N-N--0.415700        0    -7.00163  -5.70669   6.32306  L
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C-CT--0.001400       -1   -6.2637   -6.55716   7.25185  L
C-C-0.597300         0    -4.7607   -6.51455   6.95494  L
O-O--0.567900        0    -4.3273   -6.67053   5.80747  L
C-CT--0.015200       0    -6.76713  -8.01113   7.1678   L
C-CA--0.001100       0    -8.26774  -8.17395   7.00897  L
C-CA--0.190600       0    -9.10956  -8.3458    8.1271   L
C-CA--0.190600       0    -8.8212   -8.10279   5.71761  L
C-CA--0.234100       0    -10.50492  -8.46112   7.94829  L
C-CA--0.234100       0    -10.20927  -8.19343   5.54516  L
C-C-0.322600         0    -11.05542  -8.38872   6.65072  L
O-OH--0.557900       0    -12.39173  -8.51133   6.44373  L
H-H-0.271900         0    -6.72304  -5.73536   5.34665  L
H-H1-0.087600        0    -6.42711  -6.19332   8.26743  L
H-HC-0.029500        0    -6.43846  -8.54602   8.05951  L
H-HC-0.029500        0    -6.29391  -8.49556   6.31194  L
H-HA-0.169900        0    -8.68653  -8.37447   9.12067  L
H-HA-0.169900        0    -8.18354  -7.93486   4.85917  L
H-HA-0.165600        0    -11.16656  -8.59325   8.78968  L
H-HA-0.165600        0    -10.63515  -8.07925   4.56644  L
H-HO-0.399200        0    -12.5381  -8.59953   5.48951  L
N-N--0.516300        0    -3.9515   -6.31851   7.99346  L
C-CT-0.039700        -1   -2.501    -6.25075   7.85983  L
C-C-0.536600         0    -1.81811  -7.62795   7.91853  L
O-O--0.581900        0    -2.03208  -8.41716   8.83859  L
C-CT-0.056000        0    -1.8757   -5.27548   8.8656   L
C-CT-0.013600        0    -2.12118  -3.81386   8.45874  L
C-C-0.805400         0    -3.59296  -3.37816   8.56482  L
O-O2--0.818800       0    -4.2983   -3.8718    9.47861  L
O-O2--0.818800       0    -4.02228  -2.53826   7.74277  L
H-H-0.293600         0    -4.35638  -6.02559   8.87464  L
H-H1-0.110500        0    -2.29482  -5.84459   6.87605  L
H-HC--0.017300       0    -0.79547  -5.43288   8.87018  L
H-HC--0.017300       0    -2.24724  -5.46936   9.87283  L
H-HC--0.042500       0    -1.76931  -3.67488   7.43463  L
H-HC--0.042500       0    -1.50142  -3.1822    9.09519  L
N-N--0.415700        0    -0.94637  -7.90798   6.94331  L
C-CT--0.002400       -1   -0.20342  -9.16869   6.81322  L
C-C-0.597300         0     1.30319  -8.95737   6.98661  L
O-O--0.567900        0     1.83561  -7.8436    7.03116  L
C-CT--0.034300       0    -0.5613   -9.82389   5.45972  L
C-CA-0.011800        0     0.00795  -9.12511   4.23238  L
C-CA--0.125600       0    -0.70119  -8.08675   3.6026   L
C-CA--0.125600       0     1.27443  -9.48738   3.73923  L
C-CA--0.170400       0    -0.11411  -7.36882   2.5434   L
C-CA--0.170400       0     1.86519  -8.76967   2.68344  L
C-CA--0.107200       0     1.17105  -7.70363   2.0886   L
H-H-0.271900         0    -0.81662  -7.19748   6.22788  L
H-H1-0.097800        0    -0.53162  -9.84494   7.60345  L
H-HC-0.029500        0    -1.64817  -9.86876   5.36811  L
H-HC-0.029500        0    -0.20458  -10.85415   5.46663  L
H-HA-0.133000        0    -1.67912  -7.80096   3.9667   L
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H-HA-0.133000        0     1.7994   -10.31275   4.18803  L
H-HA-0.143000        0    -0.63442  -6.53086   2.10111  L
H-HA-0.143000        0     2.85136  -9.03081   2.33265  L
H-HA-0.129700        0     1.61937  -7.12993   1.29075  L
N-N--0.415700        0     2.02094  -10.07205   7.10458  L
C-CT--0.024900       -1    3.46559  -10.04798   7.29044  L
C-C-0.597300         0     4.22162  -9.54633   6.04294  L
O-O--0.567900        0     4.08847  -10.09146   4.94945  L
C-CT-0.211700        0     3.99057  -11.4382   7.69247  L
O-OH--0.654600       0     3.73003  -12.44441   6.71973  L
H-H-0.271900         0     1.52813  -10.94589   7.02607  L
H-H1-0.084300        0     3.68462  -9.36707   8.11386  L
H-H1-0.035200        0     3.53343  -11.73058   8.63941  L
H-H1-0.035200        0     5.06888  -11.37131   7.84623  L
H-HO-0.427500        0     2.97075  -12.95775   7.02486  L
N-N--0.347900        0     5.08907  -8.54246   6.20099  L
C-CT--0.263700       -1    5.98159  -8.01555   5.14381  L
C-C-0.734100         0     7.05064  -9.02022   4.67831  L
O-O--0.589400        0     7.10335  -10.16236   5.13996  L
C-CT--0.000700       0     6.55908  -6.68009   5.66229  L
C-CT-0.039000        0     7.68142  -6.81484   6.70617  L
C-CT-0.048600        0     8.02375  -5.4792    7.38269  L
N-N2--0.529500       0     8.34852  -4.40092   6.42245  L
C-CA-0.807600        0     7.59485  -3.36108   6.10397  L
N-N2--0.862700       0     6.37978  -3.25066   6.54504  L
N-N2--0.862700       0     8.03107  -2.39243   5.35741  L
H-H-0.274700         0     5.09097  -8.10745   7.1102   L
H-H1-0.156000        0     5.36026  -7.79498   4.27298  L
H-HC-0.032700        0     5.74186  -6.09384   6.08691  L
H-HC-0.032700        0     6.95165  -6.11006   4.82913  L
H-HC-0.028500        0     8.57846  -7.19969   6.22396  L
H-HC-0.028500        0     7.37847  -7.52099   7.47985  L
H-H1-0.068700        0     8.88675  -5.63909   8.03098  L
H-H1-0.068700        0     7.192    -5.18452   8.02412  L
H-H-0.345600         0     9.28384  -4.40583   6.02334  L
H-H-0.447800         0     5.83974  -2.40509   6.3173   L
H-H-0.447800         0     5.96858  -3.92562   7.14626  L
H-H-0.447800         0     7.37575  -1.61295   5.25463  L
H-H-0.447800         0     8.93631  -2.38587   4.91556  L
N-N--0.415700        0     7.9203   -8.57997   3.77594  L
C-CT--0.051800       -1    9.25404  -9.12596   3.51065  L
C-C-0.597300         0     10.18726  -7.93207   3.70802  L
O-O--0.567900        0     10.23032  -7.01394   2.89379  L
C-CT--0.110200       0     9.26988  -9.74029   2.09571  L
C-CT-0.353100        0     10.59458  -10.40102   1.6616   L
C-CT--0.412100       0     10.30733  -11.46195   0.59629  L
C-CT--0.412100       0     11.5872  -9.41922   1.04115  L
H-H-0.271900         0     7.73901  -7.66111   3.37774  L
H-H1-0.092200        0     9.50286  -9.90206   4.23702  L
H-HC-0.045700        0     8.97843  -8.99142   1.35793  L
H-HC-0.045700        0     8.50433  -10.51065   2.08986  L
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H-HC--0.036100       0     11.05487  -10.88917   2.52083  L
H-HC-0.100000        0     11.23908  -11.9383    0.28939  L
H-HC-0.100000        0     9.84302   -10.99873  -0.27646  L
H-HC-0.100000        0     9.64665   -12.2292    0.99711  L
H-HC-0.100000        0     12.4769   -9.95612    0.71429  L
H-HC-0.100000        0     11.88804  -8.66521    1.76062  L
H-HC-0.100000        0     11.13439  -8.92654    0.18207  L
N-N--0.415700        0     10.87863  -7.89983    4.84112  L
C-CT-0.014300        -1    12.16881  -7.23701    4.87675  L
C-C-0.597300         0     13.18732  -8.30721    4.40099  L
O-O--0.567900        0     13.1652   -9.40515    4.95778  L
C-CT--0.204100       0     12.53128  -6.78294    6.3013   L
C-C-0.713000         0     11.73916  -5.59747    6.8129   L
O-O--0.593100        0     11.08925  -4.85794    6.09079  L
N-N--0.919100        0     11.76954  -5.36874    8.10434  L
H-H-0.271900         0     10.79978  -8.706      5.44281  L
H-H1-0.104800        0     12.20006  -6.38438    4.19647  L
H-HC-0.079700        0     13.58367  -6.4951     6.30943  L
H-HC-0.079700        0     12.41089  -7.62136    6.98786  L
H-H-0.419600         0     11.29661  -4.54436    8.42234  L
H-H-0.419600         0     12.3461   -5.93895    8.70152  L
N-N--0.415700        0     14.01803  -8.05585    3.37827  L
C-CT--0.051800       -1    15.108    -8.97504    2.99619  L
C-C-0.597300         0     16.32781  -8.78378    3.93601  L
O-O--0.567900        0     16.61085  -7.65526    4.33504  L
C-CT--0.110200       0     15.47491  -8.81072    1.48698  L
C-CT-0.353100        0     16.47505  -9.84666    0.89249  L
C-CT--0.412100       0     15.96001  -11.28115   1.05817  L
C-CT--0.412100       -1    16.75392  -9.66597   -0.61998  L
H-H-0.271900         0     13.99975  -7.15165    2.93034  L
H-H1-0.092200        0     14.74424  -9.99131    3.14312  L
H-HC-0.045700        0     15.89385  -7.81617    1.33954  L
H-HC-0.045700        0     14.55721  -8.8611     0.90297  L
H-HC--0.036100       0     17.42236  -9.75912    1.41981  L
H-HC-0.100000        0     14.97926  -11.38362   0.59423  L
H-HC-0.100000        0     15.89678  -11.54472   2.11138  L
H-HC-0.100000        0     16.65517  -11.97533   0.58505  L
H-HC-0.100000        0     15.85204  -9.86349   -1.19536  L
H-HC-0.100000        0     17.54274  -10.35055  -0.93199  L
H-HC-0.100000        0     17.09285  -8.64498   -0.79974  L
N-N--0.516300        0     17.04482  -9.8572     4.30509  L
C-CT-0.039700        -1    18.30197  -9.75477    5.0853   L
C-C-0.536600         0     19.39339  -8.95279    4.31802  L
O-O--0.581900        0     19.32156  -8.80476    3.09489  L
C-CT-0.056000        0     18.81758  -11.13421   5.5384   L
C-CT-0.013600        0     18.51234  -11.39768   7.02354  L
C-C-0.805400         0     19.04804  -10.2981    7.96277  L
O-O2--0.818800       0     18.4568   -10.13729   9.05097  L
O-O2--0.818800       0     19.98623  -9.5728     7.55051  L
H-H-0.293600         0     16.78178  -10.76249   3.9578   L
H-H1-0.110500        0     18.07408  -9.15183    5.96485  L
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H-HC--0.017300       0     19.89753  -11.18998   5.39373  L
H-HC--0.017300       0     18.36587  -11.92019   4.93046  L
H-HC--0.042500       0     18.951   -12.35818   7.30283  L
H-HC--0.042500       0     17.42847  -11.4792    7.13798  L
N-N--0.415700        0     20.36925  -8.35666    5.02156  L
C-CT--0.025200       -1    21.38396  -7.42365    4.46719  L
C-C-0.597300         0     20.77963  -6.13461    3.84055  L
O-O--0.567900        0     21.53313  -5.35881    3.25668  L
H-H-0.271900         0     20.38981  -8.58762    6.01944  L
H-H1-0.069800        0     21.95497  -7.93766    3.69412  L
H-H1-0.069800        0     22.06877  -7.12821    5.26122  L
N-N--0.415700        0     19.4568   -5.8725     3.92914  L
C-CT--0.038900       0     18.73109  -4.94373    3.02081  L
C-C-0.597300         0     17.78202  -3.93954    3.7171   L
O-O--0.567900        0     16.95624  -4.28801    4.55857  L
C-CT-0.365400        0     17.92079  -5.73812    1.9744   L
O-OH--0.676100       0     18.67825  -6.76088    1.36775  L
C-CT--0.243800       0     17.45676  -4.86586    0.80615  L
H-H-0.271900         0     18.8945   -6.53869    4.44326  L
H-H1-0.100700        0     19.47274  -4.36773    2.46879  L
H-H1-0.004300        0     17.04542  -6.17481    2.44836  L
H-HC-0.064200        0     16.80897  -4.06579    1.15498  L
H-HC-0.064200        0     16.89884  -5.48151    0.10036  L
H-HC-0.064200        0     18.32143  -4.44016    0.29633  L
H-HO-0.410200        0     18.90569  -7.43285    2.03834  L
N-N--0.415700        0     17.84011  -2.66163    3.31381  L
C-CT--0.087500       -1    16.94651  -1.55214    3.7379   L
C-C-0.597300         0     15.57867  -1.66057    3.02642  L
O-O--0.567900        0     15.52676  -1.65678    1.79994  L
C-CT-0.298500        0     17.55738  -0.18249    3.35157  L
C-CT--0.319200       -1    16.70573   1.02306    3.84293  L
C-CT--0.319200       -1    19.00628  -0.11067    3.86666  L
H-H-0.271900         0     18.52329  -2.45627    2.60013  L
H-H1-0.096900        0     16.80636  -1.59463    4.81729  L
H-HC--0.029700       0     17.61264  -0.11624    2.26463  L
H-HC-0.079100        0     16.58537   0.98259    4.92455  L
H-HC-0.079100        0     15.73165   1.02959    3.35444  L
H-HC-0.079100        0     17.22571   1.94352    3.57932  L
H-HC-0.079100        0     19.03451  -0.30164    4.93959  L
H-HC-0.079100        0     19.408    0.88493    3.67541  L
H-HC-0.079100        0     19.64528  -0.82688    3.35068  L
N-N--0.415700        0     14.45834  -1.76351    3.7605   L
C-CT--0.023700       -1    13.14771  -2.17227    3.18895  L
C-C-0.597300         0     11.88857  -1.51832    3.83979  L
O-O--0.567900        0     10.76707  -2.02853    3.72921  L
C-CT-0.034200        0     13.01663  -3.70417    3.3993   L
C-CT-0.001800        0     14.08637  -4.62204    2.78525  L
S-S--0.273700        0     13.59363  -5.47823    1.26549  L
C-CT--0.053600       0     13.72714  -4.11213    0.08725  L
H-H-0.271900         0     14.60157  -1.85682    4.75342  L
H-H1-0.088000        0     13.11357  -1.95641    2.12046  L
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 H-HC-0.024100        0     12.04949  -4.04462   3.02673  L
 H-HC-0.024100        0     13.02373  -3.88334   4.47497  L
 H-H1-0.044000        0     14.32616  -5.3831    3.52691  L
 H-H1-0.044000        0     15.00836  -4.08185   2.59906  L
 H-H1-0.068400        0     14.73453  -3.69663   0.11025  L
 H-H1-0.068400        0     13.0114  -3.33177   0.3408   L
 H-H1-0.068400        0     13.5154  -4.48601  -0.91186  L
 N-N--0.415700        0     12.03914  -0.37978   4.52371  L
 C-CT--0.024900       -1    10.93821   0.56224   4.82798  L
 C-C-0.597300         0     11.04543   1.66883   3.78187  L
 O-O--0.567900        0     12.15239   2.15266   3.53817  L
 C-CT-0.211700        0     11.06798   1.08876   6.25408  L
 O-OH--0.654600       0     10.14394   2.11932   6.52605  L
 H-H-0.271900         0     12.96632   0.01833   4.4822   L
 H-H1-0.084300        0     9.97047   0.07061   4.72483  L
 H-H1-0.035200        0     12.07531   1.47194   6.39903  L
 H-H1-0.035200        0     10.90156   0.26599   6.9505   L
 H-HO-0.427500        0     9.25913   1.86551   6.18315  L
 N-N--0.347900        0     9.95001   2.01359   3.09239  L
 C-CT--0.240000       -1    10.00681   2.93458   1.94165  L
 C-C-0.734100         0     10.58854   4.29957   2.37694  L
 O-O--0.589400        0     11.59961   4.69468   1.80307  L
 C-CT--0.009400       0     8.64802   2.99369   1.216    L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.65446   3.62154  -0.19745  H
 C-CT--0.047900       0     7.44284   3.11119  -0.99844  H
 C-CT--0.014300       0     7.15607   3.89168  -2.27535  H
 N-N3--0.385400       0     5.92095   3.36832  -2.98119  H
 H-H-0.274700         0     9.06464   1.61065   3.38386  L
 H-H1-0.142600        0     10.7287   2.52477   1.23297  L
 H-HC-0.036200        0     7.95209   3.54839   1.83434  L
 H-HC-0.036200        0     8.27792   1.96988   1.12943  L
 H-HC-0.010300        0     9.58767   3.3577   -0.7024   H
 H-HC-0.010300        0     8.62112   4.70985  -0.08194  H
 H-HC-0.062100        0     6.53796   3.16078  -0.39406  H
 H-HC-0.062100        0     7.58581   2.05705  -1.25665  H
 H-HP-0.113500        0     7.95986   3.86326  -3.01663  H
 H-HP-0.113500        0     6.94032   4.9373   -2.05298  H
 H-H-0.340000         0     6.13121   2.63521  -3.67286  H
 H-H-0.340000         0     5.48842   4.09655  -3.58679  H
 H-H-0.340000         0     5.17972   3.00691  -2.32586  H
 N-N--0.347900        0     10.11033   4.91076   3.48477  L
 C-CT--0.263700       -1    10.70832   6.08226   4.21619  L
 C-C-0.734100         0     11.98913   5.78291   4.98614  L
 O-O--0.589400        0     12.25909   6.36826   6.03167  L
 C-CT--0.000700       0     9.60565   6.78504   5.0457   L
 C-CT-0.039000        0     8.54395   7.40786   4.11476  L
 C-CT-0.048600        0     7.45385   8.23813   4.81206  L
 N-N2--0.529500       0     6.6072    7.46206   5.74262  L
 C-CA-0.807600        0     5.36896   7.75375   6.107    L
 N-N2--0.862700       0     4.62671   8.63708   5.52071  L
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N-N2--0.862700       0     4.81579   7.14687   7.11091  L
H-H-0.274700         0     9.26323   4.50245   3.86263  L
H-H1-0.156000        0     11.03787   6.8022    3.46125  L
H-HC-0.032700        0     10.04838   7.59068   5.63363  L
H-HC-0.032700        0     9.13984   6.06942   5.72495  L
H-HC-0.028500        0     8.06725   6.62878   3.52729  L
H-HC-0.028500        0     9.05537   8.06544   3.4121   L
H-H1-0.068700        0     6.82708   8.67631   4.0331   L
H-H1-0.068700        0     7.9276    9.0561    5.35722  L
H-H-0.345600         0     7.00577   6.68342   6.24697  L
H-H-0.447800         0     3.69019   8.77445   5.88802  L
H-H-0.447800         0     4.82342   9.00806   4.59796  L
H-H-0.447800         0     3.85864   7.40702   7.34576  L
H-H-0.447800         0     5.26736   6.35899   7.54401  L
N-N--0.347900        0     12.78849   4.88307   4.41446  L
C-CT--0.240000       -1    14.18185   4.57036   4.73374  L
C-C-0.734100         0     15.0348   4.24321   3.47807  L
O-O--0.589400        0     16.25413   4.27886   3.58043  L
C-CT--0.009400       0     14.2997   3.46832   5.81243  L
C-CT-0.018700        0     13.53988   3.86145   7.09061  L
C-CT--0.047900       0     13.74955   2.96747   8.31372  L
C-CT--0.014300       0     12.75843   3.47876   9.37128  L
N-N3--0.385400       0     12.8785   2.76549   10.66551  L
H-H-0.274700         0     12.40347   4.51153   3.55903  L
H-H1-0.142600        0     14.63634   5.47516   5.14329  L
H-HC-0.036200        0     15.3547   3.33479   6.05767  L
H-HC-0.036200        0     13.91516   2.52507   5.42671  L
H-HC-0.010300        0     12.47299   3.86283   6.8659   L
H-HC-0.010300        0     13.8432   4.87083   7.37243  L
H-HC-0.062100        0     14.77887   3.06612   8.66363  L
H-HC-0.062100        0     13.53851   1.92796   8.06196  L
H-HP-0.113500        0     11.74333   3.36963   8.97151  L
H-HP-0.113500        0     12.93421   4.5503    9.51621  L
H-H-0.340000         0     12.69079   1.77951   10.54468  L
H-H-0.340000         0     12.20881   3.13964   11.32741  L
H-H-0.340000         0     13.80768   2.88376   11.04823  L
N-N--0.415700        0     14.43138   3.92883   2.31848  L
C-CT--0.051800       -1    15.07484   3.50224   1.04828  L
C-C-0.597300         0     15.2968   4.61377   0.05822  L
O-O--0.567900        0     16.2566   4.58227  -0.70948  L
C-CT--0.110200       0     14.2086   2.36102   0.47308  L
C-CT-0.353100        0     14.73171   1.69666  -0.81558  L
C-CT--0.412100       0     16.1154   1.07084  -0.63606  L
C-CT--0.412100       0     13.76331   0.58751  -1.23583  L
H-H-0.271900         0     13.42158   3.93193   2.32385  L
H-H1-0.092200        0     16.05946   3.09786   1.28838  L
H-HC-0.045700        0     13.21213   2.75689   0.27043  L
H-HC-0.045700        0     14.10898   1.58869   1.23788  L
H-HC--0.036100       0     14.7729   2.43413  -1.61647  L
H-HC-0.100000        0     16.10385   0.35882   0.18816  L
H-HC-0.100000        0     16.85344   1.84745  -0.43763  L
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H-HC-0.100000        0     16.40739   0.55531  -1.55061  L
H-HC-0.100000        0     14.10088   0.14687  -2.17376  L
H-HC-0.100000        0     12.76688   1.00263  -1.38274  L
H-HC-0.100000        0     13.72613  -0.18814  -0.46962  L
N-N--0.415700        0     14.41573   5.59996   0.08556  L
C-CT-0.014300        -1    14.6294    6.81355  -0.65494  L
C-C-0.597300         0     15.72346   7.72575  -0.02665  L
O-O--0.567900        0     15.44874   8.83429   0.42525  L
C-CT--0.204100       0     13.26755   7.50589  -0.92339  L
C-C-0.713000         0     12.33067   7.71441   0.26495  L
O-O--0.593100        0     12.65249   7.5162    1.42755  L
N-N--0.919100        0     11.09658   8.08119  -0.00664  L
H-H-0.271900         0     13.67134   5.58933   0.77265  L
H-H1-0.104800        0     15.02046   6.54531  -1.63808  L
H-HC-0.079700        0     12.72662   6.90564  -1.65408  L
H-HC-0.079700        0     13.45423   8.48071  -1.37274  L
H-H-0.419600         0     10.50108   8.24755   0.78223  L
H-H-0.419600         0     10.75308   8.20045  -0.95611  L
N-N--0.415700        0     16.98568   7.26194  -0.0556   L
C-CT--0.149000       -1    18.19355   7.93885   0.43557  L
H-H-0.271900         0     17.08207   6.32451  -0.43245  L
H-H1-0.097600        0     18.13712   8.04351   1.52048  L
H-H1-0.097600        0     18.26327   8.93339  -0.00905  L
H-H1-0.097600        0     19.08052   7.36092   0.17311  L
C-CT--0.055800       0     3.04841   13.69567   4.61461  L
C-CT-0.000000        0     3.11149   13.0765    3.21752  L
O-OS--0.354800       0     4.45269   13.1015    2.73839  L
C-CT--0.202200       0     2.67915   11.61585   3.25986  L
O-OS--0.524600       0     1.98913   11.31493   2.04467  L
C-CT--0.067000       0     4.00803   10.90364   3.42751  L
O-OH--0.613900       0     3.88997   9.58891    2.94376  L
C-CT--0.006600       0     4.91815   11.76652   2.5769   L
N-N*--0.048400       0     6.34979   11.60758   2.96045  L
C-C-0.753800         0     7.18629   10.80497   2.17306  L
O-O--0.625200        0     6.77138   10.24971   1.16104  L
N-NC--0.758400       0     8.48718   10.62358   2.51675  L
C-CA-0.818500        0     8.94257   11.22349   3.59032  L
N-N2--0.953000       0     10.20021   11.00928   3.85088  L
C-CM--0.521500       0     8.1436    12.02306   4.44939  L
C-CM--0.005300       0     6.84376   12.19708   4.09851  L
H-H1-0.067900        0     2.01639   13.6799    4.96774  L
H-H1-0.067900        0     3.66817   13.12148   5.30228  L
H-H1-0.117400        0     2.43575   13.63112   2.56253  L
H-H1-0.061500        0     2.03664   11.44292   4.11972  L
H-H1-0.097200        0     4.30771   10.94937   4.47517  L
H-HO-0.418600        0     3.02268   9.59182    2.49481  L
H-H2-0.202900        0     4.75705   11.45331   1.5491   L
H-H-0.423400         0     10.68477   10.49023   3.1414   L
H-H-0.423400         0     10.64957   11.48218   4.60855  L
H-HA-0.192800        0     8.53145   12.50196   5.33284  L
H-H4-0.195800        0     6.18203   12.81173   4.69872  L
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 P-P-1.166200          0     0.61434   10.43463   1.98955  L
 O-O2--0.776000        0    -0.27574   10.9281    0.9206   L
 O-O2--0.776000        0     0.10722   10.15221   3.35369  L
 O-OS--0.498900        0     1.25328   9.0816     1.4615   L
 C-CT-0.055800         0     1.81106   9.00622    0.17101  L    H-H1
1581  0.        0.
 C-CT-0.106500         0     2.32618   7.588     -0.05665  H
 O-OS--0.354800        0     3.18693   7.2495     1.03238  H
 C-CT-0.202200         0     1.23558   6.50989   -0.16105  H
 O-OH--0.654100        0     1.07729   6.01573   -1.47074  H
 C-CT-0.067000         0     1.72464   5.35058    0.77971  H
 O-OH--0.613900        0     2.32473   4.24281    0.16924  H
 C-CT-0.039400         0     2.83693   6.01508    1.61011  H
 N-N*--0.025100        0     2.53473   6.159      3.02692  H
 C-CK-0.200600         0     1.55847   6.88724    3.69443  H
 N-NB--0.607300        0     1.48465   6.61489    4.9709   H
 C-CB-0.051500         0     2.4304    5.63262    5.16727  H
 C-CA-0.700900         0     2.78081   4.84376    6.28315  H
 N-N2--0.901900        0     2.24385   5.03602    7.51651  H
 N-NC--0.761500        0     3.76716   3.93987    6.14907  H
 C-CQ-0.587500         0     4.24518   3.70993    4.92874  H
 N-NC--0.699700        0     4.01203   4.38938    3.81374  H
 C-CB-0.305300         0     3.08662   5.33974    3.97855  H
 H-H1-0.067900         0     2.64156   9.70655    0.1014   L
 H-H1-0.067900         0     1.05819   9.25215   -0.58227  L
 H-H1-0.117400         0     2.89386   7.58729   -0.99313  H
 H-H1-0.061500         0     0.2783    6.8915     0.22247  H
 H-HO-0.437600         0     0.78269   6.70927   -2.10411  H
 H-H1-0.097200         0     0.90395   5.06846    1.44561  H
 H-HO-0.418600         0     5.24046   4.12534    0.86723  H
 H-H2-0.200700         0     3.69599   5.3593     1.55483  H
 H-H5-0.155300         0     0.92721   7.60162    3.18176  H
 H-H-0.411500          0     2.23159   4.19033    8.09859  H
 H-H-0.411500          0     1.33984   5.4996     7.52622  H
 H-H5-0.047300         0     4.96848   2.90762    4.83693  H
 N-N3-0.149300         0    -0.64077   4.11133   -0.36263  H
 C-CT-0.053600         0     0.13453   3.02547    0.28316  H
 C-CT-0.065100         0    -0.57385   1.67347    0.08964  H
 C-CT--0.090300        0    -0.63585   0.8166     1.36592  H
 C-C-0.735400          0    -1.68792  -0.28005    1.24521  H
 O-O--0.613300         0    -1.42356  -1.44847    1.02399  H
 N-N--1.003100         0    -2.98307   0.18091    1.28561  H
 C-C-0.612300          0     1.53945   3.0757    -0.36817  H
 O-O--0.571300         0     1.5989    2.94208   -1.60522  H
 O-OS--0.421200        0     2.30969   1.9026     0.38833  H
 P-P-1.166200          0     3.76537   1.43305    0.06411  H
 O-O2--0.776000        0     4.57142   1.32596    1.41715  H
 O-O2--0.776000        0     4.54405   2.19342   -0.9821   H
 O-OS--0.498900        0     3.74636  -0.1221    -0.29683  H
 C-CT-0.055800         0     2.97205  -0.55114   -1.42388  H
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 C-CT-0.106500        0     2.38923  -1.95326  -1.15367  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.37114  -2.90556  -0.73387  L
 C-CT-0.039400        0     3.2377   -3.12311   0.67435  L
 N-N*--0.025100       0     4.57315  -3.08995   1.32399  L
 C-CB-0.305300        0     5.32543  -4.2029    1.60967  L
 N-NC--0.699700       0     4.96248  -5.50311   1.42419  L
 C-CQ-0.587500        0     5.90619  -6.34335   1.81462  L
 N-NC--0.761500       0     7.09925  -6.0657    2.32424  L
 C-CA-0.700900        0     7.42914  -4.77916   2.44627  L
 N-N2--0.901900       0     8.66141  -4.59763   2.88593  L
 C-CB-0.051500        0     6.51868  -3.75011   2.10656  L
 N-NB--0.607300       0     6.54557  -2.35118   2.154    L
 C-CK-0.200600        0     5.35113  -2.02254   1.7179   L
 C-CT-0.067000        0     2.19886  -2.13635   1.21521  L
 O-OH--0.613900       0     1.46174  -2.65267   2.31096  L
 C-CT-0.202200        0     1.34673  -1.94284  -0.04597  L
 O-OH--0.654100       0     0.43523  -3.02001  -0.23953  L
 H-H-0.199600         0    -1.89757   3.70243  -1.43741  H
 H-H-0.199600         0    -0.05329   4.63013  -1.01263  H
 H-H-0.199600         0    -1.0139    4.76535   0.32258  H
 H-HP-0.101500        0     0.21987   3.22334   1.35957  H
 H-HC-0.005000        0    -0.09801   1.12487  -0.72943  H
 H-HC-0.005000        0    -1.59737   1.88669  -0.23279  H
 H-HC-0.033100        0    -0.89934   1.45746   2.21827  H
 H-HC-0.033100        0     0.32582   0.35769   1.59375  H
 H-H-0.442900         0    -3.70606  -0.50142   1.45463  H
 H-H-0.442900         0    -3.14026   1.06948   1.76636  H
 H-H1-0.067900        0     3.61603  -0.5943   -2.30905  H
 H-H1-0.067900        0     2.15427   0.14375  -1.61611  H
 H-H1-0.117400        0     1.90336  -2.28258  -2.07225  L
 H-H2-0.200700        0     2.80915  -4.11448   0.82996  L
 H-H5-0.047300        0     5.66949  -7.39154   1.70622  L
 H-H-0.411500         0     9.03308  -3.66376   2.95064  L
 H-H-0.411500         0     9.24591  -5.42645   2.93838  L
 H-H5-0.155300        0     5.01732  -0.99799   1.63501  L
 H-H1-0.097200        0     2.65975  -1.18986   1.49502  L
 H-HO-0.418600        0     2.02993  -2.67387   3.1061   L
 H-H1-0.061500        0     0.81854  -0.9935   -0.04005  L
 H-HO-0.437600        0    -0.33242  -2.76751   0.31686  L
 O-OW--0.834000       0    -10.31091  -2.12555   11.56839  L
 H-HW-0.417000        0    -10.60776  -1.27144   11.17265  L
 H-HW-0.417000        0    -10.613   -2.77076   10.90477  L
 O-OW--0.834000       0    -10.31736  -3.87492   9.4808   L
 H-HW-0.417000        0    -10.57238  -3.21962   8.80358  L
 H-HW-0.417000        0    -9.68933  -4.43856   8.98943  L
 O-OW--0.834000       0    -10.75355  -1.93072   7.673    L
 H-HW-0.417000        0    -11.54613  -1.52301   8.10623  L
 H-HW-0.417000        0    -10.10442  -1.22532   7.76815  L
 O-OW--0.834000       0     5.46315   3.69856   1.71943  H
 H-HW-0.417000        0     4.80887   4.04238   2.40005  H
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H-HW-0.417000        0     4.96348   2.23775   1.59578  H
O-OW--0.834000       0     6.9913    4.35494   4.085    H
H-HW-0.417000        0     6.7854    3.94058   3.22599  H
H-HW-0.417000        0     6.50224   5.19186   3.93926  H
O-OW--0.834000       0     6.46936   2.22068  -5.4501   L
H-HW-0.417000        0     7.36614   2.00079  -5.77332  L
H-HW-0.417000        0     6.22406   2.98563  -5.9862   L
O-OW--0.834000       0     6.49331   4.72704   6.83265  L
H-HW-0.417000        0     5.62673   4.29323   6.92398  L
H-HW-0.417000        0     6.76293   4.48392   5.93206  L
O-OW--0.834000       0     7.79136   1.49268   5.25662  H
H-HW-0.417000        0     7.18688   2.24039   5.12842  H
H-HW-0.417000        0     7.14912   0.77655   5.51716  H
O-OW--0.834000       0     5.64782   6.74019   2.53083  H
H-HW-0.417000        0     4.92124   7.38467   2.42902  H
H-HW-0.417000        0     5.65095   6.30968   1.65486  H
O-OW--0.834000       0     5.76603   15.30447   3.77966  L
H-HW-0.417000        0     5.3025    14.55134   3.3842   L
H-HW-0.417000        0     5.08133   15.96764   3.87249  L
O-OW--0.834000       0    -4.26429   2.13077   5.5384   L
H-HW-0.417000        0    -4.08121   2.02902   6.47681  L
H-HW-0.417000        0    -4.73712   3.00573   5.52701  L
O-OW--0.834000       0     0.31998   1.72683   12.18709  L
H-HW-0.417000        0    -0.0475    1.44577   13.04741  L
H-HW-0.417000        0     0.03495   2.64437   12.15704  L
O-OW--0.834000       0    -1.89682   9.61583   5.73942  L
H-HW-0.417000        0    -1.86613   8.74164   6.18528  L
H-HW-0.417000        0    -1.41793   9.47271   4.90856  L
O-OW--0.834000       0     2.20266   8.44878   6.93734  L
H-HW-0.417000        0     1.71951   7.80955   6.38046  L
H-HW-0.417000        0     1.67848   9.2665    6.78785  L
O-OW--0.834000       0    -4.62451   9.07037   5.64373  L
H-HW-0.417000        0    -4.61339   8.17119   6.03256  L
H-HW-0.417000        0    -3.71656   9.38369   5.7876   L
O-OW--0.834000       0    -2.19681   7.26746   7.07063  L
H-HW-0.417000        0    -3.07994   6.88292   6.86091  L
H-HW-0.417000        0    -2.03736   6.96144   7.98061  L
O-OW--0.834000       0     0.7044    10.45127   5.95336  L
H-HW-0.417000        0     0.65709   10.44773   4.97109  L
H-HW-0.417000        0    -0.23719   10.42704   6.18692  L
N-N                  0     5.86705   7.97859  -0.39287  H
H-H                  0     6.24121   8.03273   0.54753  H
H-H                  0     5.71728   8.82823  -0.91119  H
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**TS2**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.82336 | -11.25648 | -5.73693 | L |
| C-C-0.597200 | 0 | -12.13797 | -10.22535 | -6.60429 | L |
| O-O--0.567900 | 0 | -11.7734 | -10.54738 | -7.72631 | L |
| H-HC-0.112300 | 0 | -12.20762 | -11.44919 | -4.8613 | L |
| H-HC-0.112300 | 0 | -12.93502 | -12.17453 | -6.31187 | L |
| H-HC-0.112300 | 0 | -13.8036 | -10.88439 | -5.44732 | L |
| N-N--0.415700 | 0 | -11.93193 | -9.02095 | -6.06243 | L |
| C-CT--0.058100 | -1 | -11.05177 | -7.99401 | -6.64125 | L |
| C-C-0.597300 | 0 | -10.01528 | -7.52198 | -5.61712 | L |
| O-O--0.567900 | 0 | -10.28672 | -7.47958 | -4.4109 | L |
| C-CT--0.007400 | 0 | -11.83906 | -6.86178 | -7.29727 | L |
| C-CC-0.186800 | 0 | -11.21233 | -6.33559 | -8.56323 | L |
| N-NB--0.543200 | 0 | -11.58515 | -6.69627 | -9.85749 | L |
| C-CW--0.220700 | 0 | -10.33459 | -5.29617 | -8.62663 | L |
| C-CR-0.163500 | 0 | -10.97725 | -5.81756 | -10.66799 | L |
| N-NA--0.279500 | 0 | -10.22308 | -4.96277 | -9.95899 | L |
| H-H-0.271900 | 0 | -12.28501 | -8.84277 | -5.13797 | L |
| H-H1-0.136000 | 0 | -10.49415 | -8.47594 | -7.44625 | L |
| H-HC-0.036700 | 0 | -11.91193 | -6.03947 | -6.59493 | L |
| H-HC-0.036700 | 0 | -12.84633 | -7.20246 | -7.54106 | L |
| H-H4-0.186200 | 0 | -9.92248 | -4.75463 | -7.7899 | L |
| H-H-0.333900 | 0 | -9.85814 | -4.07759 | -10.33144 | L |
| H-H5-0.143500 | 0 | -11.13503 | -5.75436 | -11.73535 | L |
| N-N--0.415700 | 0 | -8.81961 | -7.19153 | -6.09943 | L |
| C-CT--0.038900 | -1 | -7.65026 | -6.72593 | -5.3321 | L |
| C-C-0.597300 | 0 | -6.86241 | -5.63634 | -6.09802 | L |
| O-O--0.567900 | 0 | -7.19892 | -5.3009 | -7.23318 | L |
| C-CT-0.365400 | 0 | -6.67855 | -7.88058 | -5.01078 | L |
| O-OH--0.676100 | 0 | -6.41111 | -8.63527 | -6.15427 | L |
| C-CT--0.243800 | -1 | -7.20239 | -8.84296 | -3.96154 | L |
| H-H-0.271900 | 0 | -8.6724 | -7.36589 | -7.0878 | L |
| H-H1-0.100700 | 0 | -7.96022 | -6.31588 | -4.37749 | L |
| H-H1-0.004300 | 0 | -5.74043 | -7.4732 | -4.63375 | L |
| H-HC-0.064200 | 0 | -7.46396 | -8.29556 | -3.05585 | L |
| H-HC-0.064200 | 0 | -6.43461 | -9.57731 | -3.72294 | L |
| H-HC-0.064200 | 0 | -8.08807 | -9.35533 | -4.3381 | L |
| H-HO-0.410200 | 0 | -5.71181 | -9.28107 | -5.96234 | L |
| N-N--0.347900 | 0 | -5.78647 | -5.07307 | -5.51208 | L |
| C-CT--0.263700 | -1 | -4.77955 | -4.24027 | -6.221 | L |
| C-C-0.734100 | 0 | -3.38801 | -4.30834 | -5.60004 | L |
| O-O--0.589400 | 0 | -3.28775 | -4.46794 | -4.38849 | L |
| C-CT--0.000700 | 0 | -5.25836 | -2.78381 | -6.37809 | L |
| C-CT-0.039000 | 0 | -5.0794 | -1.8544 | -5.1651 | L |
| C-CT-0.048600 | 0 | -5.94731 | -2.15719 | -3.94656 | L |
| N-N2--0.529500 | 0 | -5.36665 | -3.18572 | -3.07201 | L |
| C-CA-0.807600 | 0 | -5.49379 | -3.27578 | -1.76604 | L |
| N-N2--0.862700 | 0 | -6.33101 | -2.55161 | -1.08572 | L |
| N-N2--0.862700 | 0 | -4.73333 | -4.12111 | -1.13362 | L |
| H-H-0.274700 | 0 | -5.56616 | -5.38541 | -4.57766 | L |
| H-H1-0.156000 | 0 | -4.69898 | -4.66563 | -7.21837 | L |

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 H-HC-0.032700        0    -6.30532  -2.77276  -6.68525  L
 H-HC-0.032700        0    -4.68986  -2.34391  -7.19846  L
 H-HC-0.028500        0    -5.36795  -0.86423  -5.48921  L
 H-HC-0.028500        0    -4.03212  -1.79853  -4.87281  L
 H-H1-0.068700        0    -6.94052  -2.4518   -4.28097  L
 H-H1-0.068700        0    -6.03252  -1.22834  -3.38039  L
 H-H-0.345600         0    -4.64695  -3.77099  -3.47053  L
 H-H-0.447800         0    -6.4588   -2.6393   -0.08724  L
 H-H-0.447800         0    -7.03091  -1.98156  -1.57989  L
 H-H-0.447800         0    -4.54231  -3.96152  -0.14851  L
 H-H-0.447800         0    -4.16351  -4.76362  -1.66803  L
 N-N--0.415700        0    -2.32123  -4.0774   -6.36116  L
 C-CT--0.002400      -1    -1.07261  -3.54705  -5.78535  L
 C-C-0.597300         0    -1.1564   -2.01811  -5.76769  L
 O-O--0.567900        0    -1.32393  -1.44754  -6.84802  L
 C-CT--0.034300       0     0.13982  -4.039    -6.58522  L
 C-CA-0.011800        0     1.4591   -3.46428  -6.09588  L
 C-CA--0.125600       0     1.9036   -3.7037   -4.77985  L
 C-CA--0.125600       0     2.24332  -2.67419  -6.95649  L
 C-CA--0.170400       0     3.10429  -3.12579  -4.32707  L
 C-CA--0.170400       0     3.43645  -2.09013  -6.50124  L
 C-CA--0.107200       0     3.85755  -2.29883  -5.17919  L
 H-H-0.271900         0    -2.50693  -3.95881  -7.35324  L
 H-H1-0.097800        0    -0.95248  -3.92395  -4.77142  L
 H-HC-0.029500        0    -0.00095  -3.77701  -7.63528  L
 H-HC-0.029500        0     0.18891  -5.12624  -6.51377  L
 H-HA-0.133000        0     1.32319  -4.32393  -4.11107  L
 H-HA-0.133000        0     1.92516  -2.4995   -7.97084  L
 H-HA-0.143000        0     3.44708  -3.3085   -3.32002  L
 H-HA-0.143000        0     4.02349  -1.47311  -7.16643  L
 H-HA-0.129700        0     4.76284  -1.82375  -4.82694  L
 N-N--0.254800        0    -1.10726  -1.36028  -4.59152  L
 C-CT--0.026600       0    -1.23823   0.08688  -4.49268  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.12683   0.80433  -4.30758  H
 O-O--0.574800        0     0.54975   1.14051  -3.21054  H
 C-CT--0.007000       0    -2.16106   0.28542  -3.28804  L
 C-CT-0.018900        0    -1.70639  -0.81874  -2.33105  L
 C-CT-0.019200        0    -1.28476  -1.95176  -3.26702  L
 H-H1-0.064100        0    -1.7389    0.46632  -5.3698   L
 H-HC-0.025300        0    -3.19644   0.11373  -3.58498  L
 H-HC-0.025300        0    -2.0601    1.27666  -2.85161  L
 H-HC-0.021300        0    -2.51574  -1.12705  -1.66844  L
 H-HC-0.021300        0    -0.84619  -0.48792  -1.75076  L
 H-H1-0.039100        0    -0.35931  -2.40852  -2.91614  L
 H-H1-0.039100        0    -2.082    -2.69029  -3.28571  L
 N-N--0.254800        0     0.89561   1.05554  -5.40458  H
 C-CT--0.026600       0     2.14473   1.76144  -5.19667  H
 C-C-0.589600         0     1.91904   3.24307  -4.86883  H
 O-O--0.574800        0     0.98158   3.88077  -5.32038  H
 C-CT--0.007000       0     2.84029   1.68927  -6.56965  H
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 C-CT-0.018900        0     1.65714   1.65251  -7.53877  H
 C-CT-0.019200        0     0.6768    0.73501  -6.81594  H
 H-H1-0.064100        0     2.72322   1.29326  -4.39302  H
 H-HC-0.025300        0     3.43428   0.77478  -6.63744  H
 H-HC-0.025300        0     3.50664   2.54094  -6.7311   H
 H-HC-0.021300        0     1.91136   1.28111  -8.53209  H
 H-HC-0.021300        0     1.22911   2.65184  -7.62713  H
 H-H1-0.039100        0    -0.3548    0.90593  -7.11737  H
 H-H1-0.039100        0     0.92852  -0.31303  -7.0122   H
 N-N--0.415700        0     2.93269   3.74485  -4.1227   H
 C-CT-0.039700        0     3.28383   5.1467   -3.98374  H
 C-C-0.597300         0     4.25029   5.52985  -5.15369  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.31552   4.91202  -5.24767  L
 C-CT--0.003600       0     3.78671   5.31545  -2.52758  H
 C-CT-0.013600        0     4.8741    6.34703  -2.25357  H
 C-C-0.805400         0     5.47901   6.19304  -0.8634   H
 O-O2--0.818800       0     5.50063   5.1298   -0.23577  H
 H-H-0.271900         0     3.62541   3.09792  -3.77702  H
 H-H1-0.110500        0     2.36307   5.71664  -4.11082  H
 H-HC--0.017300       0     2.90175   5.51005  -1.92109  H
 H-HC--0.017300       0     4.12096   4.35732  -2.12358  H
 H-HC--0.042500       0     4.52179   7.37667  -2.36892  H
 H-HC--0.042500       0     5.71781   6.25405  -2.95158  H
 N-N--0.254800        0     3.89063   6.45043  -6.09181  L
 C-CT--0.026600      -1     4.69416   6.79971  -7.28977  L
 C-C-0.589600         0     6.11398   7.30117  -6.96632  L
 O-O--0.574800        0     6.99424   7.22252  -7.82246  L
 C-CT--0.007000       0     3.86569   7.75429  -8.14814  L
 C-CT-0.018900        0     2.63943   8.11338  -7.3106   L
 C-CT-0.019200        0     2.60371   7.1354   -6.13579  L
 H-H1-0.064100        0     4.82069   5.8863   -7.86632  L
 H-HC-0.025300        0     3.54705   7.23711  -9.05366  L
 H-HC-0.025300        0     4.43116   8.64158  -8.4276   L
 H-HC-0.021300        0     1.73615   8.01655  -7.91112  L
 H-HC-0.021300        0     2.72624   9.13355  -6.94147  L
 H-H1-0.039100        0     2.4203    7.68266  -5.20928  L
 H-H1-0.039100        0     1.80529   6.40857  -6.29533  L
 N-N--0.415700        0     6.38907   7.75581  -5.73809  L
 C-CT-0.014300       -1     7.75178   7.91739  -5.2339   L
 C-C-0.597300         0     8.52557   6.60795  -5.18846  L
 O-O--0.567900        0     8.29589   5.74401  -4.34163  L
 C-CT--0.204100       0     7.7433    8.60793  -3.85906  L
 C-C-0.713000         0     9.15226   8.89769  -3.36346  L
 O-O--0.593100        0     9.76169   8.14413  -2.61981  L
 N-N--0.919100        0     9.74036   9.98969  -3.78365  L
 H-H-0.271900         0     5.61058   7.95528  -5.11099  L
 H-H1-0.104800        0     8.26934   8.58868  -5.92197  L
 H-HC-0.079700        0     7.24325   7.97876  -3.12745  L
 H-HC-0.079700        0     7.19956   9.54523  -3.93652  L
 H-H-0.419600         0     10.65472   10.17367  -3.41874  L
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H-H-0.419600          0     9.25566   10.64642  -4.39275  L
N-N--0.415700         0     9.52805   6.52923   -6.05099  L
C-CT--0.025200        -1    10.70795   5.73974  -5.78612  L
C-C-0.597300          0     11.02985   4.75315  -6.91298  L
O-O--0.567900         0     11.51543   5.12602  -7.97594  L
H-H-0.271900          0     9.55487   7.20011   -6.80567  L
H-H1-0.069800         0     10.61242   5.19651  -4.84543  L
H-H1-0.069800         0     11.55829   6.41441  -5.68871  L
N-N--0.415700         0     10.77206   3.4812   -6.63273  L
C-CT--0.001400        -1    10.78043   2.30818  -7.51796  L
C-C-0.597300          0     9.70275   1.37626   -6.93696  L
O-O--0.567900         0     8.86111   1.81809   -6.14382  L
C-CT--0.015200        0     12.20393   1.70975  -7.55234  L
C-CA--0.001100        0     12.67227   1.33053  -8.94321  L
C-CA--0.190600        0     13.07495   2.34766  -9.83117  L
C-CA--0.190600        0     12.7257  -0.01769  -9.34816  L
C-CA--0.234100        0     13.53867   2.02242  -11.12037  L
C-CA--0.234100        0     13.17791  -0.34629  -10.64075  L
C-C-0.322600          0     13.58779   0.67114  -11.52671  L
O-OH--0.557900        0     14.02104   0.34857  -12.77309  L
H-H-0.271900          0     10.28385   3.33187  -5.76199  L
H-H1-0.087600         0     10.47924   2.60779  -8.52365  L
H-HC-0.029500         0     12.27712   0.85045  -6.88487  L
H-HC-0.029500         0     12.9145   2.44701   -7.17428  L
H-HA-0.169900         0     13.0241   3.38319   -9.51622  L
H-HA-0.169900         0     12.42633  -0.80764  -8.6746   L
H-HA-0.165600         0     13.84591   2.80736  -11.79338  L
H-HA-0.165600         0     13.21789  -1.37432  -10.96712  L
H-HO-0.399200         0     14.30176   1.12558  -13.25638  L
N-N--0.415700         0     9.77781   0.0804   -7.19367  L
C-CT--0.051800        -1    9.31196  -0.92131  -6.23612  L
C-C-0.597300          0     10.44969  -1.88675  -5.95387  L
O-O--0.567900         0     11.40591  -2.00506  -6.72014  L
C-CT--0.110200        0     8.00485  -1.56305  -6.7528   L
C-CT-0.353100         0     8.07061  -2.28388  -8.11738  L
C-CT--0.412100        0     8.58346  -3.72267  -7.99663  L
C-CT--0.412100        0     6.66579  -2.34792  -8.71725  L
H-H-0.271900          0     10.43028  -0.21945  -7.90682  L
H-H1-0.092200         0     9.10359  -0.41042  -5.30421  L
H-HC-0.045700         0     7.27365  -0.75618  -6.82417  L
H-HC-0.045700         0     7.6255   -2.26369  -6.01048  L
H-HC--0.036100        0     8.70732  -1.7336   -8.80876  L
H-HC-0.100000         0     9.6272   -3.72811  -7.69261  L
H-HC-0.100000         0     8.51501  -4.21459  -8.96698  L
H-HC-0.100000         0     7.98882  -4.27722  -7.27136  L
H-HC-0.100000         0     5.99373  -2.88928  -8.05716  L
H-HC-0.100000         0     6.69656  -2.83722  -9.69179  L
H-HC-0.100000         0     6.28223  -1.34092  -8.85534  L
N-N--0.415700         0     10.37747  -2.52824  -4.8026   L
C-CT--0.058100        -1    11.45195  -3.35205  -4.2695   L
C-C-0.597300          0     10.92713  -4.7427   -3.93802  L
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 O-O--0.567900        0     9.72426  -4.99419  -3.93176  L
 C-CT--0.007400       0     12.06208  -2.62897  -3.05308  L
 C-CC-0.186800        0     11.07244  -2.28541  -1.95941  L
 N-NB--0.543200       0     10.5872  -3.16533  -0.99229  L
 C-CW--0.220700       0     10.45451  -1.07915  -1.80427  L
 C-CR-0.163500        0     9.68379  -2.47075  -0.27944  L
 N-NA--0.279500       0     9.57301  -1.22019  -0.75242  L
 H-H-0.271900         0     9.53654  -2.39128  -4.24991  L
 H-H1-0.136000        0     12.23185  -3.47678  -5.02263  L
 H-HC-0.036700        0     12.52108  -1.70228  -3.40029  L
 H-HC-0.036700        0     12.8574  -3.24088  -2.63346  L
 H-H4-0.186200        0     10.58543  -0.21552  -2.44027  L
 H-H-0.333900         0     8.86139  -0.56244  -0.45523  L
 H-H5-0.143500        0     9.08475  -2.86866   0.53018  L
 N-N--0.415700        0     11.82581  -5.68287  -3.6644   L
 C-CT--0.059700       -1    11.41102  -7.0583   -3.38583  L
 C-C-0.597300         0     10.49074  -7.19845  -2.14755  L
 O-O--0.567900        0     9.70971  -8.14421  -2.06215  L
 C-CT-0.130300        0     12.62934  -7.99462  -3.31361  L
 C-CT--0.043000       0     12.14354  -9.45822  -3.25899  L
 C-CT--0.320400       0     13.56589  -7.655    -2.13898  L
 C-CT--0.066000       -1    13.18727  -10.44555  -3.76086  L
 H-H-0.271900         0     12.80714  -5.4564   -3.70391  L
 H-H1-0.086900        0     10.82067  -7.38154  -4.24081  L
 H-HC-0.018700        0     13.19    -7.85947  -4.24072  L
 H-HC-0.023600        0     11.26646  -9.57603  -3.8962   L
 H-HC-0.023600        0     11.8637  -9.72486  -2.23896  L
 H-HC-0.088200        0     14.45622  -8.27869  -2.18976  L
 H-HC-0.088200        0     13.06837  -7.83061  -1.18458  L
 H-HC-0.088200        0     13.88733  -6.61579  -2.18804  L
 H-HC-0.018600        0     12.77388  -11.45402  -3.72913  L
 H-HC-0.018600        0     14.07532  -10.41104  -3.13017  L
 H-HC-0.018600        0     13.46216  -10.2087  -4.7893   L
 N-N--0.415700        0     10.52526  -6.24692  -1.20819  L
 C-CT--0.025200       -1    9.5096   -6.11729  -0.16267  L
 C-C-0.597300         0     8.11095  -5.97111  -0.75657  L
 O-O--0.567900        0     7.283    -6.8735   -0.61918  L
 H-H-0.271900         0     11.15256  -5.46737  -1.34069  L
 H-H1-0.069800        0     9.73109  -5.25853   0.46675  L
 H-H1-0.069800        0     9.5226   -7.01068   0.45698  L
 N-N--0.415700        0     7.87073  -4.87304  -1.48418  L
 C-CT--0.058100       0     6.6607   -4.6768   -2.29628  L    H-HC
246   0.        0.
 C-C-0.597300         0     6.30135  -5.9188   -3.11426  L
 O-O--0.567900        0     5.12747  -6.26829  -3.19627  L
 C-CT--0.007400       0     6.82977  -3.52464  -3.28333  H
 C-CC-0.186800        0     6.94852  -2.11282  -2.81848  H
 N-NB--0.543200       0     7.79619  -1.30177  -3.52678  H
 C-CW--0.220700       0     6.17794  -1.35459  -1.97426  H
 C-CR-0.163500        0     7.4904   -0.07366  -3.17199  H
 N-NA--0.279500       0     6.53809  -0.05374  -2.21259  H
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H-H-0.271900          0     8.6413   -4.22626  -1.60931  L
H-H1-0.136000         0     5.8133   -4.45924  -1.64338  L
H-HC-0.036700         0     5.96933  -3.5727   -3.96018  H
H-HC-0.036700         0     7.69328  -3.71752  -3.9157   H
H-H4-0.186200         0     5.4017   -1.57488  -1.26459  H
H-H-0.333900          0     5.98215   0.76266  -1.94563  H
H-H5-0.143500         0     7.92427   0.83842  -3.57489  H
N-N--0.415700         0     7.29156  -6.5928   -3.70951  L
C-CT-0.033700         -1    7.08277  -7.80917  -4.48719  L
C-C-0.597300          0     6.26743  -8.89079  -3.77133  L
O-O--0.567900         0     5.43027  -9.53112  -4.40653  L
C-CT--0.182500        0     8.39048  -8.33808  -5.08032  L
H-H-0.271900          0     8.22261  -6.19495  -3.64971  L
H-H1-0.082300         0     6.47074  -7.51274  -5.33705  L
H-HC-0.060300         0     8.94652  -7.52215  -5.54337  L
H-HC-0.060300         0     8.1601   -9.08045  -5.84569  L
H-HC-0.060300         0     8.98903  -8.8202   -4.31289  L
N-N--0.347900         0     6.43492  -9.06841  -2.45577  L
C-CT--0.240000        -1    5.53338  -9.92461  -1.67493  L
C-C-0.734100          0     4.0653   -9.4452   -1.71789  L
O-O--0.589400         0     3.17585  -10.27133  -1.90293  L
C-CT--0.009400        0     6.05205  -10.10165  -0.23746  L
C-CT-0.018700         0     5.16271  -11.06504   0.57495  L
C-CT--0.047900        0     5.79162  -11.40643   1.93024  L
C-CT--0.014300        0     4.8221   -12.1909   2.82296  L
N-N3--0.385400        0     5.40648  -12.43858   4.16626  L
H-H-0.274700          0     7.12688  -8.48459  -1.99108  L
H-H1-0.142600         0     5.52893  -10.90859  -2.14737  L
H-HC-0.036200         0     6.08666  -9.13338   0.26281  L
H-HC-0.036200         0     7.0658   -10.50356  -0.28361  L
H-HC-0.010300         0     5.01268  -11.9879   0.01232  L
H-HC-0.010300         0     4.19298  -10.59656   0.7468   L
H-HC-0.062100         0     6.05173  -10.4735   2.42837  L
H-HC-0.062100         0     6.69475  -11.99575   1.76496  L
H-HP-0.113500         0     4.55251  -13.13229   2.33566  L
H-HP-0.113500         0     3.91108  -11.59292   2.93561  L
H-H-0.340000          0     4.68568  -12.70784   4.8318   L
H-H-0.340000          0     5.7746   -11.56285   4.53811  L
H-H-0.340000          0     6.1484   -13.12022   4.14713  L
N-N--0.415700         0     3.7998   -8.14477  -1.54465  L
C-CT--0.024900        -1    2.46019  -7.53791  -1.70803  L
C-C-0.597300          0     1.896    -7.76134  -3.12208  L
O-O--0.567900         0     0.75707  -8.2093   -3.22947  L
C-CT-0.211700         0     2.46913  -6.03861  -1.35624  L
O-OH--0.654600        0     1.14007  -5.5568   -1.27509  L
H-H-0.271900          0     4.59945  -7.52815  -1.48571  L
H-H1-0.084300         0     1.78097  -8.03121  -1.01195  L
H-H1-0.035200         0     3.01593  -5.47243  -2.10984  L
H-H1-0.035200         0     2.95156  -5.90359  -0.38997  L
H-HO-0.427500         0     1.12108  -4.63126  -0.97014  L
N-N--0.415700         0     2.67394  -7.52454  -4.19575  L
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C-CT--0.059700       -1    2.33279  -7.90488  -5.59281  L
C-C-0.597300         0     1.89148  -9.38658  -5.60536  L
O-O--0.567900        0     0.75789  -9.67501  -5.96844  L
C-CT-0.130300        0     3.48771  -7.61992  -6.58375  L
C-CT--0.043000       0     3.88924  -6.12925  -6.55265  L
C-CT--0.320400       0     3.08329  -8.01976  -8.0151   L
C-CT--0.066000       0     5.12644  -5.79019  -7.39017  L
H-H-0.271900         0     3.58632  -7.12088  -4.0094   L
H-H1-0.086900        0     1.47135  -7.31214  -5.90264  L
H-HC-0.018700        0     4.35132  -8.2172   -6.29776  L
H-HC-0.023600        0     4.1074   -5.8313   -5.52974  L
H-HC-0.023600        0     3.05478  -5.52566  -6.90596  L
H-HC-0.088200        0     2.2613   -7.39389  -8.36426  L
H-HC-0.088200        0     2.77749  -9.06525  -8.05932  L
H-HC-0.088200        0     3.92698  -7.89997  -8.6942   L
H-HC-0.018600        0     4.87309  -5.77271  -8.45027  L
H-HC-0.018600        0     5.9184   -6.51744  -7.21866  L
H-HC-0.018600        0     5.48475  -4.80658  -7.09536  L
N-N--0.415700        0     2.73939  -10.32419  -5.1619   L
C-CT-0.021300        -1    2.48872  -11.77783  -5.20429  L
C-C-0.597300         0     1.25764  -12.27647  -4.44905  L
O-O--0.567900        0     0.67937  -13.286   -4.83703  L
C-CT--0.123100       -1    3.78582  -12.54994  -4.81492  L
S-SH--0.311900       0     5.12911  -12.21048  -5.9893   L
H-H-0.271900         0     3.65176  -10.01236  -4.85234  L
H-H1-0.112400        0     2.28313  -12.02994  -6.24659  L
H-H1-0.111200        0     3.57049  -13.62034  -4.83261  L
H-H1-0.111200        0     4.09113  -12.26899  -3.8062   L
H-HS-0.193300        0     5.32306  -10.93042  -5.63835  L
N-N--0.415700        0     0.8516   -11.59471  -3.38237  L
C-CT--0.051800       -1   -0.38737  -11.8974  -2.67157  L
C-C-0.597300         0    -1.60528  -11.21012  -3.31641  L
O-O--0.567900        0    -2.59637  -11.88825  -3.56312  L
C-CT--0.110200       0    -0.22849  -11.46709  -1.20219  L
C-CT-0.353100        0     0.78014  -12.32975  -0.41856  L
C-CT--0.412100       0     1.13827  -11.64235   0.89701  L
C-CT--0.412100       0     0.22098  -13.71556  -0.08883  L
H-H-0.271900         0     1.41602  -10.80476  -3.09483  L
H-H1-0.092200        0    -0.58119  -12.97022  -2.70848  L
H-HC-0.045700        0    -1.19874  -11.52661  -0.70703  L
H-HC-0.045700        0     0.09308  -10.42405  -1.17939  L
H-HC--0.036100       0     1.69879  -12.45149  -0.99153  L
H-HC-0.100000        0     1.59712  -10.68055   0.67255  L
H-HC-0.100000        0     1.84092  -12.25409   1.45796  L
H-HC-0.100000        0     0.23692  -11.47747   1.48924  L
H-HC-0.100000        0     0.94787  -14.28301   0.48993  L
H-HC-0.100000        0     0.01548  -14.26177  -1.00913  L
H-HC-0.100000        0    -0.70379  -13.62121   0.4813   L
N-N--0.415700        0    -1.55461  -9.90048  -3.61094  L
C-CT-0.014300        -1   -2.64873  -9.17582  -4.28764  L
C-C-0.597300         0    -3.02317  -9.82361  -5.6064   L
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O-O--0.567900        0    -4.18036  -10.1891  -5.81546  L
C-CT--0.204100       0    -2.37672  -7.66535  -4.36263  L
C-C-0.713000         0    -2.57451  -6.98727  -3.01218  L
O-O--0.593100        0    -3.67289  -6.63098  -2.60692  L
N-N--0.919100        0    -1.51951  -6.78537  -2.2625   L
H-H-0.271900         0    -0.6904   -9.4057   -3.42383  L
H-H1-0.104800        0    -3.53995  -9.29731  -3.66673  L
H-HC-0.079700        0    -3.09326  -7.219    -5.05076  L
H-HC-0.079700        0    -1.37538  -7.47316  -4.74564  L
H-H-0.419600         0    -1.64461  -6.28115  -1.40538  L
H-H-0.419600         0    -0.60629  -7.09098  -2.57133  L
N-N--0.415700        0    -2.01753  -10.0504  -6.43992  L
C-CT--0.002400      -1    -2.17814  -10.83973  -7.63995  L
C-C-0.597300         0    -2.39965  -12.33499  -7.42967  L
O-O--0.567900        0    -2.91164  -13.00834  -8.31827  L
C-CT--0.034300       0    -1.03932  -10.55389  -8.63438  L
C-CA-0.011800        0    -1.14646  -9.18477  -9.28957  L
C-CA--0.125600       0    -1.88485  -9.0374   -10.47982  L
C-CA--0.125600       0    -0.56725  -8.04774  -8.69308  L
C-CA--0.170400       0    -2.05758  -7.76587  -11.05622  L
C-CA--0.170400       0    -0.73001  -6.77715  -9.27581  L
C-CA--0.107200       0    -1.48376  -6.63435  -10.45293  L
H-H-0.271900         0    -1.0862   -9.74018  -6.18847  L
H-H1-0.097800        0    -3.09283  -10.49924  -8.12863  L
H-HC-0.029500        0    -1.07485  -11.30309  -9.42674  L
H-HC-0.029500        0    -0.07343  -10.66193  -8.14365  L
H-HA-0.133000        0    -2.35086  -9.89748  -10.93935  L
H-HA-0.133000        0    -0.0176   -8.14403  -7.77255  L
H-HA-0.143000        0    -2.65695  -7.65117  -11.95002  L
H-HA-0.143000        0    -0.29822  -5.90394  -8.81293  L
H-HA-0.129700        0    -1.63914  -5.65603  -10.88767  L
N-N--0.415700        0    -2.05904  -12.84485  -6.2523   L
C-CT--0.025200      -1    -2.29618  -14.22152  -5.85237  L
C-C-0.597300         0    -3.76323  -14.61292  -5.71369  L
O-O--0.567900        0    -4.1389   -15.73255  -6.04787  L
H-H-0.271900         0    -1.66281  -12.22303  -5.56629  L
H-H1-0.069800        0    -1.80961  -14.40021  -4.89437  L
H-H1-0.069800        0    -1.84165  -14.88505  -6.58848  L
N-N--0.415700        0    -4.58014  -13.70123  -5.18841  L
C-CT--0.059700      -1    -6.04267  -13.8348  -5.1228   L
C-C-0.597300         0    -6.7106   -13.74834  -6.49859  L
O-O--0.567900        0    -7.74237  -14.38174  -6.71503  L
C-CT-0.130300        0    -6.57854  -12.80364  -4.07536  L
C-CT--0.043000       0    -6.25215  -13.33158  -2.6375   L
C-CT--0.320400      -1    -8.08903  -12.45054  -4.21478  L
C-CT--0.066000      -1    -5.55333  -12.35591  -1.66124  L
H-H-0.271900         0    -4.15193  -12.83637  -4.88043  L
H-H1-0.086900        0    -6.28285  -14.8348  -4.7594   L
H-HC-0.018700        0    -6.02957  -11.87291  -4.22807  L
H-HC-0.023600        0    -5.60263  -14.20499  -2.70754  L
H-HC-0.023600        0    -7.17482  -13.67814  -2.17023  L
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H-HC-0.088200        0    -8.27005  -11.94851  -5.16732  L
H-HC-0.088200        0    -8.3879   -11.77855  -3.41036  L
H-HC-0.088200        0    -8.6906   -13.35927  -4.17332  L
H-HC-0.018600        0    -4.59892  -12.03562  -2.06975  L
H-HC-0.018600        0    -5.38763  -12.84982  -0.70369  L
H-HC-0.018600        0    -6.18859  -11.48323  -1.51181  L
N-N--0.415700        0    -6.10293  -13.01084  -7.43108  L
C-CT--0.149000       -1   -6.51328  -12.96332  -8.82238  L
H-H-0.271900         0    -5.2484   -12.54903  -7.16211  L
H-H1-0.097600        0    -6.81331  -13.95856  -9.15568  L
H-H1-0.097600        0    -5.68509  -12.61288  -9.4395   L
H-H1-0.097600        0    -7.36114  -12.28279  -8.92789  L
C-CT--0.366200       -1   -8.90195  -9.73773  -10.90334  L
C-C-0.597200         0    -8.13798  -9.08606  -9.81627  L
O-O--0.567900        0    -8.4866   -9.12378  -8.6439   L
H-HC-0.112300        0    -8.27575  -10.45987  -11.42183  L
H-HC-0.112300        0    -9.27683  -8.97713  -11.58646  L
H-HC-0.112300        0    -9.75424  -10.24999  -10.45521  L
N-N--0.415700        0    -7.06841  -8.47223  -10.26483  L
C-CT-0.021300        -1   -6.25729  -7.63356  -9.44014  L
C-C-0.597300         0    -5.74682  -6.46587  -10.28286  L
O-O--0.567900        0    -5.14961  -6.70396  -11.33629  L
C-CT--0.123100       0    -5.06807  -8.45444  -8.91792  L
S-SH--0.311900       0    -3.96045  -7.40337  -7.92215  L
H-H-0.271900         0    -6.88684  -8.47273  -11.2556  L
H-H1-0.112400        0    -6.83505  -7.25638  -8.59764  L
H-H1-0.111200        0    -4.51464  -8.86517  -9.76185  L
H-H1-0.111200        0    -5.44147  -9.2824   -8.31492  L
H-HS-0.193300        0    -3.46     -6.69698  -8.949    L
N-N--0.415700        0    -5.94417  -5.22673  -9.82965  L
C-CT-0.014300        -1   -5.46764  -4.05181  -10.55477  L
C-C-0.597300         0    -4.10013  -3.51867  -10.04631  L
O-O--0.567900        0    -3.50538  -4.02918  -9.09154  L
C-CT--0.204100       0    -6.58971  -2.99976  -10.66103  L
C-C-0.713000         0    -6.37714  -2.00668  -11.80261  L
O-O--0.593100        0    -5.54215  -2.19551  -12.67714  L
N-N--0.919100        0    -7.06162  -0.89756  -11.81977  L
H-H-0.271900         0    -6.46603  -5.10783  -8.96628  L
H-H1-0.104800        0    -5.2738   -4.3684   -11.58127  L
H-HC-0.079700        0    -6.69583  -2.45975  -9.72065  L
H-HC-0.079700        0    -7.52301  -3.51805  -10.87109  L
H-H-0.419600         0    -6.93442  -0.28265  -12.59415  L
H-H-0.419600         0    -7.83861  -0.76182  -11.15796  L
N-N--0.415700        0    -3.57014  -2.48335  -10.69792  L
C-CT--0.051800       -1   -2.36597  -1.74052  -10.33457  L
C-C-0.597300         0    -2.76277  -0.26408  -10.03604  L
O-O--0.567900        0    -3.09206   0.47165  -10.96401  L
C-CT--0.110200       0    -1.34293  -1.85112  -11.48331  L
C-CT-0.353100        0    -0.0904   -0.96938  -11.30599  L
C-CT--0.412100       0     0.7359   -1.38593  -10.09042  L
C-CT--0.412100       0     0.80862  -1.07238  -12.53779  L
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H-H-0.271900          0    -4.0982   -2.14259  -11.49779  L
H-H1-0.092200         0    -1.92872  -2.16455  -9.43039  L
H-HC-0.045700         0    -1.8377   -1.55312  -12.40977  L
H-HC-0.045700         0    -1.03956  -2.89381  -11.58593  L
H-HC--0.036100        0    -0.37934   0.07414  -11.19056  L
H-HC-0.100000         0     1.01336  -2.43634  -10.17717  L
H-HC-0.100000         0     0.15571  -1.2345   -9.18124  L
H-HC-0.100000         0     1.63565  -0.77455  -10.03081  L
H-HC-0.100000         0     1.14655  -2.10019  -12.67145  L
H-HC-0.100000         0     1.66883  -0.41593  -12.41532  L
H-HC-0.100000         0     0.24937  -0.7595   -13.41989  L
N-N--0.347900         0    -2.73954   0.18948  -8.76679  L
C-CT--0.263700        -1   -3.45408   1.40695  -8.29081  L
C-C-0.734100          0    -2.55038   2.45281  -7.64745  L
O-O--0.589400         0    -2.19525   2.35334  -6.48156  L
C-CT--0.000700        0    -4.58425   0.96549  -7.35422  L
C-CT-0.039000         0    -5.69582   2.01571  -7.21342  L
C-CT-0.048600         0    -6.54742   1.71688  -5.97638  L
N-N2--0.529500        0    -5.84514   2.14732  -4.75327  L
C-CA-0.807600         0    -6.2007    1.95712  -3.50342  L
N-N2--0.862700        0    -7.27988   1.35133  -3.13884  L
N-N2--0.862700        0    -5.45463   2.37323  -2.54355  L
H-H-0.274700          0    -2.36761  -0.44133  -8.06334  L
H-H1-0.156000         0    -3.92962   1.88164  -9.15167  L
H-HC-0.032700         0    -4.15092   0.74312  -6.37912  L
H-HC-0.032700         0    -5.04273   0.05486  -7.74388  L
H-HC-0.028500         0    -6.32764   1.98452  -8.10252  L
H-HC-0.028500         0    -5.27084   3.017    -7.12199  L
H-H1-0.068700         0    -6.78515   0.65442  -5.93925  L
H-H1-0.068700         0    -7.49568   2.2367   -6.06393  L
H-H-0.345600          0    -5.03754   2.77122  -4.83467  L
H-H-0.447800          0    -7.50221   1.30567  -2.15584  L
H-H-0.447800          0    -7.87993   0.88017  -3.79342  L
H-H-0.447800          0    -5.70226   2.18199  -1.58503  L
H-H-0.447800          0    -4.59791   2.88766  -2.76768  L
N-N--0.415700         0    -2.15637   3.45451  -8.41826  L
C-CT--0.002400        -1   -1.29599   4.52197  -7.91928  L
C-C-0.597300          0    -2.01708   5.40608  -6.89878  L
O-O--0.567900         0    -3.04706   5.99799  -7.20406  L
C-CT--0.034300        0    -0.76665   5.34387  -9.10171  L
C-CA-0.011800         0     0.22355   4.58667  -9.97037  L
C-CA--0.125600        0     1.60566   4.75911  -9.76897  L
C-CA--0.125600        0    -0.22729   3.6992   -10.96773  L
C-CA--0.170400        0     2.52972   4.06303  -10.56815  L
C-CA--0.170400        0     0.69625   2.98474  -11.75112  L
C-CA--0.107200        0     2.07563   3.1691   -11.55444  L
H-H-0.271900          0    -2.52635   3.51311  -9.35108  L
H-H1-0.097800         0    -0.44268   4.07438  -7.41376  L
H-HC-0.029500         0    -0.27532   6.23621  -8.71     L
H-HC-0.029500         0    -1.60458   5.68103  -9.7146   L
H-HA-0.133000         0     1.9522    5.43511  -9.00153  L
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 H-HA-0.133000        0    -1.28595   3.56067  -11.13722  L
 H-HA-0.143000        0     3.58686   4.22044  -10.4226   L
 H-HA-0.143000        0     0.33626   2.3036   -12.5099   L
 H-HA-0.129700        0     2.78095   2.62859  -12.16747  L
 N-N--0.516300        0    -1.43682   5.51025   -5.70483  L
 C-CT-0.038100        0    -1.94167   6.32427   -4.60153  L    H-HC
515   0.        0.
 C-C-0.536600         0    -1.03649   7.5596    -4.43052  L
 O-O--0.581900        0    -0.23481   7.6589    -3.49369  L
 C-CT--0.030300       0    -2.01484   5.45116   -3.3445   H
 C-C-0.799400         0    -3.06415   4.34784   -3.36385  H
 O-O2--0.801400       0    -3.05045   3.57303   -2.27182  H
 O-O2--0.801400       0    -3.90537   4.11923   -4.19872  H
 H-H-0.293600         0    -0.62261   4.92978   -5.53331  L
 H-H1-0.088000        0    -2.95034   6.6778    -4.82682  L
 H-HC--0.012200       0    -2.24348   6.08453   -2.47852  H
 H-HC--0.012200       0    -1.03636   4.98871   -3.17562  H
 N-N--0.516300        0    -1.15647   8.50051   -5.36868  L
 C-CT-0.038100        0    -0.32643   9.70332   -5.54719  L
 C-C-0.536600         0    -0.74948   10.89138   -4.65984  L
 O-O--0.581900        0    -0.48041   12.05236   -4.96766  L
 C-CT--0.030300       0    -0.34662   10.09241   -7.03987  L
 C-C-0.799400         0    -1.67427   10.69512   -7.52074  L
 O-O2--0.801400       0    -2.73023   10.24944   -7.01506  L
 O-O2--0.801400       0    -1.6152    11.5485   -8.43422  L
 H-H-0.293600         0    -1.91301   8.42313   -6.04635  L
 H-H1-0.088000        0     0.69882   9.45527   -5.28211  L
 H-HC--0.012200       0    -0.13993   9.20744   -7.6413   L
 H-HC--0.012200       0     0.45766   10.80832   -7.22064  L
 N-N--0.415700        0    -1.36762   10.60486   -3.50973  L
 C-CT--0.038900      -1    -2.07436   11.54497   -2.61317  L
 C-C-0.597300         0    -1.1755    12.68378   -2.02854  L
 O-O--0.567900        0    -1.66818   13.5224   -1.27823  L
 C-CT-0.365400        0    -2.75554   10.79964   -1.47445  L
 O-OH--0.676100       0    -1.88438   9.89955   -0.80597  L
 C-CT--0.243800      -1    -3.89598   10.02774   -2.11586  L
 H-H-0.271900         0    -1.46386   9.61765   -3.31846  L
 H-H1-0.100700        0    -2.84224   12.05429   -3.19581  L
 H-H1-0.004300        0    -3.16366   11.5037   -0.75071  L
 H-HC-0.064200        0    -4.57646   10.71497   -2.61787  L
 H-HC-0.064200        0    -4.42735   9.51123   -1.32335  L
 H-HC-0.064200        0    -3.52733   9.28811   -2.82641  L
 H-HO-0.410200        0    -1.2228    10.42762   -0.33476  L
 N-N--0.415700        0     0.1258    12.75862   -2.36524  L
 C-CT-0.014300       -1     1.11598   13.8155   -2.04372  L
 C-C-0.597300         0     2.08793   13.9468   -3.24275  L
 O-O--0.567900        0     3.20186   13.41649   -3.17281  L
 C-CT--0.204100       0     1.74861   13.44194   -0.69561  L
 C-C-0.713000         0     2.92135   14.29476   -0.27084  L
 O-O--0.593100        0     3.23048   15.3403   -0.82054  L
 N-N--0.919100        0     3.64058   13.83837    0.7251   L
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H-H-0.271900         0     0.36368   12.10983  -3.10767  L
H-H1-0.104800        0     0.6004    14.76595  -1.90664  L
H-HC-0.079700        0     2.07073   12.40662  -0.73031  L
H-HC-0.079700        0     0.98231   13.52131   0.07641  L
H-H-0.419600         0     4.37287   14.44478   1.03827  L
H-H-0.419600         0     3.33143   13.02008   1.24933  L
N-N--0.254800        0     1.69443   14.63947  -4.3398   L
C-CT--0.026600       -1    2.41457   14.65701  -5.62893  L
C-C-0.589600         0     3.80279   15.27958  -5.55713  L
O-O--0.574800        0     4.64026   15.05735  -6.42709  L
C-CT--0.007000       0     1.48637   15.35184  -6.63002  L
C-CT-0.018900        0     0.56478   16.19112  -5.74965  L
C-CT-0.019200        0     0.42888   15.34855  -4.48367  L
H-H1-0.064100        0     2.54493   13.62522  -5.95858  L
H-HC-0.025300        0     0.8948    14.59721  -7.15236  L
H-HC-0.025300        0     2.03157   15.96607  -7.34796  L
H-HC-0.021300        0    -0.4017    16.36362  -6.22447  L
H-HC-0.021300        0     1.0506    17.13764  -5.50834  L
H-H1-0.039100        0     0.22608   15.99578  -3.63032  L
H-H1-0.039100        0    -0.38064   14.62753  -4.6092   L
N-N--0.415700        0     4.09971   16.03627  -4.50326  L
C-CT--0.025200       -1    5.29932   16.85642  -4.43057  L
C-C-0.597300         0     6.60171   16.16786  -4.0267   L
O-O--0.567900        0     7.48542   16.76761  -3.42093  L
H-H-0.271900         0     3.41357   16.09892  -3.76455  L
H-H1-0.069800        0     5.12151   17.65355  -3.70881  L
H-H1-0.069800        0     5.46608   17.33005  -5.39876  L
N-N--0.347900        0     6.71186   14.90763  -4.41594  L
C-CT--0.240000       -1    7.84495   13.98293  -4.3201   L
C-C-0.734100         0     7.69156   12.90127  -5.41846  L
O-O--0.589400        0     8.38419   11.88473  -5.36115  L
C-CT--0.009400       0     7.85265   13.35883  -2.89867  L
C-CT-0.018700        0     6.45893   12.9128   -2.39553  L
C-CT--0.047900       0     6.4878    11.65919  -1.51276  L
C-CT--0.014300       0     5.11659   11.26472  -0.93328  L
N-N3--0.385400       0     4.06108   11.027    -1.94923  L
H-H-0.274700         0     5.87833   14.59045  -4.89736  L
H-H1-0.142600        0     8.78267   14.51133  -4.49391  L
H-HC-0.036200        0     8.24276   14.09693  -2.19585  L
H-HC-0.036200        0     8.5395    12.51222  -2.88417  L
H-HC-0.010300        0     5.83089   12.69629  -3.24709  L
H-HC-0.010300        0     6.00075   13.73494  -1.84299  L
H-HC-0.062100        0     7.16565   11.8495   -0.68017  L
H-HC-0.062100        0     6.88594   10.82238  -2.08334  L
H-HP-0.113500        0     4.79187   12.06011  -0.25983  L
H-HP-0.113500        0     5.25409   10.36045  -0.33381  L
H-H-0.340000         0     3.89565   11.8527   -2.52706  L
H-H-0.340000         0     3.16219   10.81989  -1.5384   L
H-H-0.340000         0     4.27401   10.27126  -2.60274  L
N-N--0.516300        0     6.76004   13.06133  -6.37623  L
C-CT-0.039700        -1    6.23994   11.9896   -7.24834  L
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C-C-0.536600          0      6.38881   12.33403  -8.75811  L
O-O--0.581900         0      6.1486    13.46668  -9.16426  L
C-CT-0.056000         0      4.84423   11.4848   -6.82865  L
C-CT-0.013600         0      4.83155   11.27314  -5.31001  L
C-C-0.805400          0      3.94427   10.17291  -4.73412  L
O-O2--0.818800        0      2.76892   10.44286  -4.44002  L
O-O2--0.818800        0      4.52687   9.18538   -4.22515  L
H-H-0.293600          0      6.26814   13.94382  -6.47112  L
H-H1-0.110500         0      6.89361   11.12945  -7.10497  L
H-HC--0.017300        0      4.65666   10.54024  -7.33062  L
H-HC--0.017300        0      4.07468   12.20263  -7.1122   L
H-HC--0.042500        0      4.55103   12.22501  -4.86994  L
H-HC--0.042500        0      5.84186   11.04149  -4.97507  L
N-N--0.415700         0      6.87213   11.38287  -9.5864   L
C-CT--0.149000        -1     7.25359   11.58066  -11.00349  L
H-H-0.271900          0      7.03092   10.47175  -9.18533  L
H-H1-0.097600         0      8.02979   12.34495  -11.07019  L
H-H1-0.097600         0      6.38295   11.92163  -11.5677  L
H-H1-0.097600         0      7.61993   10.64725  -11.43186  L
C-CT--0.366200        0      10.19683   1.60735  -12.31989  L
C-C-0.597200          0      9.06656   1.13478   -11.43766  L
O-O--0.567900         0      9.30575   0.77916   -10.28848  L
H-HC-0.112300         0      10.77129   2.34896  -11.76818  L
H-HC-0.112300         0      9.81898   2.04726   -13.24005  L
H-HC-0.112300         0      10.8347   0.75503   -12.5471  L
N-N--0.415700         0      7.84086   1.15033   -11.97201  L
C-CT--0.059700        -1     6.62766   0.66115   -11.29355  L
C-C-0.597300          0      5.77214  -0.19732   -12.2428  L
O-O--0.567900         0      5.80807  -1.41901   -12.14058  L
C-CT-0.130300         0      5.84947   1.79396   -10.56693  L
C-CT--0.043000        0      6.74575   2.50728   -9.51982  L
C-CT--0.320400        0      4.60633   1.21177   -9.86415  L
C-CT--0.066000        0      6.10886   3.701     -8.79961  L
H-H-0.271900          0      7.77513   1.44001   -12.93342  L
H-H1-0.086900         0      6.95625  -0.02827   -10.51617  L
H-HC-0.018700         0      5.5231    2.52815   -11.30527  L
H-HC-0.023600         0      7.63047   2.90148   -10.01676  L
H-HC-0.023600         0      7.07365   1.78283   -8.77241  L
H-HC-0.088200         0      3.9541    0.69864   -10.57025  L
H-HC-0.088200         0      4.02128   2.00835   -9.41127  L
H-HC-0.088200         0      4.90489   0.51223   -9.08398  L
H-HC-0.018600         0      5.27416   3.38145   -8.17825  L
H-HC-0.018600         0      5.7684    4.4335    -9.53122  L
H-HC-0.018600         0      6.85483   4.16998   -8.15667  L
N-N--0.415700         0      5.01746   0.41486   -13.16762  L
C-CT--0.149000        -1     4.15652  -0.2914    -14.12386  L
H-H-0.271900          0      5.03095   1.42179   -13.18206  L
H-H1-0.097600         0      3.68259  -1.14775   -13.63814  L
H-H1-0.097600         0      4.75403  -0.6574    -14.9604  L
H-H1-0.097600         0      3.37904   0.37583   -14.49934  L
C-CT--0.366200        -1    -4.83146   17.17486  -2.69651  L
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C-C-0.597200         0    -5.39749   16.37512  -1.53645  L
O-O--0.567900        0    -5.17679   16.75461  -0.38965  L
H-HC-0.112300        0    -5.64421   17.61933  -3.26598  L
H-HC-0.112300        0    -4.23519   16.51737  -3.32757  L
H-HC-0.112300        0    -4.1921    17.96101  -2.29883  L
N-N--0.254800        0    -6.17524   15.31431  -1.80621  L
C-CT--0.026600       -1   -6.85246   14.54015  -0.77194  L
C-C-0.589600         0    -5.98495   13.43    -0.18419  L
O-O--0.574800        0    -5.42796   12.58646  -0.88405  L
C-CT--0.007000       0    -8.06772   13.94668  -1.49446  L
C-CT-0.018900        0    -7.55911   13.71133  -2.91892  L
C-CT-0.019200        0    -6.58715   14.87227  -3.13434  L
H-H1-0.064100        0    -7.19845   15.1984   0.02568  L
H-HC-0.025300        0    -8.87206   14.68352  -1.51503  L
H-HC-0.025300        0    -8.41671   13.0243  -1.03079  L
H-HC-0.021300        0    -8.37261   13.72689  -3.64463  L
H-HC-0.021300        0    -7.02065   12.76488  -2.97655  L
H-H1-0.039100        0    -5.72898   14.53832  -3.71969  L
H-H1-0.039100        0    -7.10134   15.68501  -3.64842  L
N-N--0.415700        0    -5.93723   13.42069   1.14042  L
C-CT--0.023700       -1   -5.10045   12.54905   1.95155  L
C-C-0.597300         0    -5.31902   11.03051   1.76266  L
O-O--0.567900        0    -6.39075   10.57772   1.35735  L
C-CT-0.034200        0    -5.36318   12.88005   3.43461  L
C-CT-0.001800        0    -4.87857   14.27314   3.85798  L
S-S--0.273700        0    -3.08149   14.45487   4.01887  L
C-CT--0.053600       -1   -2.7865    13.51727   5.5451   L
H-H-0.271900         0    -6.43488   14.1601   1.60575  L
H-H1-0.088000        0    -4.05532   12.76378   1.71959  L
H-HC-0.024100        0    -4.8767    12.13927   4.06931  L
H-HC-0.024100        0    -6.43621   12.81238   3.62205  L
H-H1-0.044000        0    -5.32646   14.51308   4.82257  L
H-H1-0.044000        0    -5.2353    15.0109   3.13909  L
H-H1-0.068400        0    -3.04413   12.46821   5.39701  L
H-H1-0.068400        0    -3.38665   13.93013   6.35555  L
H-H1-0.068400        0    -1.73063   13.58282   5.80858  L
N-N--0.415700        0    -4.29905   10.24835   2.14348  L
C-CT--0.001400       -1   -4.16461   8.80251   1.92299  L
C-C-0.597300         0    -5.41155   7.93365   2.20704  L
O-O--0.567900        0    -6.00932   7.46353   1.24645  L
C-CT--0.015200       0    -2.87536   8.26212   2.57223  L
C-CA--0.001100       0    -2.83267   6.74807   2.73709  L
C-CA--0.190600       0    -3.16655   5.89092   1.66916  L
C-CA--0.190600       0    -2.62472   6.20358   4.01601  L
C-CA--0.234100       0    -3.32832   4.50924   1.90398  L
C-CA--0.234100       0    -2.81057   4.83055   4.25137  L
C-C-0.322600         0    -3.17017   3.97362   3.19644  L
O-OH--0.557900       0    -3.38795   2.64881   3.40976  L
H-H-0.271900         0    -3.48537   10.72224   2.50437  L
H-H1-0.087600        0    -4.00837   8.69125   0.84954  L
H-HC-0.029500        0    -2.77066   8.72072   3.55435  L
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H-HC-0.029500        0    -2.01921   8.5775    1.97392  L
H-HA-0.169900        0    -3.40141   6.31211   0.69886  L
H-HA-0.169900        0    -2.41886   6.85122   4.85428  L
H-HA-0.165600        0    -3.66225   3.84135   1.12803  L
H-HA-0.165600        0    -2.76623   4.45599   5.26154  L
H-HO-0.399200        0    -3.6691    2.49612   4.33301  L
N-N--0.516300        0    -5.76859   7.62154   3.45865  L
C-CT-0.038100        -1   -6.74228   6.55915   3.81624  L
C-C-0.536600         0    -8.13966   6.80946   3.24728  L
O-O--0.581900        0    -8.80571   5.8687    2.82601  L
C-CT--0.030300       0    -6.81024   6.40495   5.34815  L
C-C-0.799400         0    -5.5309    5.80711   5.94728  L
O-O2--0.801400       0    -5.4024    4.55931   5.92969  L
O-O2--0.801400       0    -4.66846   6.59836   6.40621  L
H-H-0.293600         0    -5.24132   8.06489   4.20573  L
H-H1-0.088000        0    -6.38699   5.61136   3.41472  L
H-HC--0.012200       0    -7.64259   5.74515   5.5969   L
H-HC--0.012200       0    -7.01349   7.37651   5.80276  L
N-N--0.415700        0    -8.56696   8.07414   3.20059  L
C-CT--0.002400       0    -9.75391   8.51342   2.46536  L
C-C-0.597300         0    -9.67343   8.1035    0.98693  L
O-O--0.567900        0    -10.54158   7.38953   0.48604  L
C-CT--0.034300       0    -9.91784   10.03284   2.62472  L
C-CA-0.011800        0    -10.97037   10.62895   1.70849  L
C-CA--0.125600       0    -12.33701   10.49708   2.01814  L
C-CA--0.125600       0    -10.58349   11.26259   0.51153  L
C-CA--0.170400       0    -13.31129   11.00107   1.13733  L
C-CA--0.170400       0    -11.55703   11.76386  -0.36991  L
C-CA--0.107200       0    -12.92152   11.63391  -0.05666  L
H-H-0.271900         0    -7.91516   8.76655   3.53787  L
H-H1-0.097800        0    -10.63234   8.02252   2.88621  L
H-HC-0.029500        0    -8.96287   10.5196   2.41973  L
H-HC-0.029500        0    -10.18187   10.25256   3.65995  L
H-HA-0.133000        0    -12.64041   9.99048   2.9232   L
H-HA-0.133000        0    -9.53616   11.33848   0.25132  L
H-HA-0.143000        0    -14.36005   10.88585   1.3706   L
H-HA-0.143000        0    -11.25236   12.22999  -1.2963   L
H-HA-0.129700        0    -13.67016   12.00716  -0.74087  L
N-N--0.415700        0    -8.63368   8.54484   0.28069  L
C-CT--0.038900       -1   -8.45699   8.26332  -1.14775  L
C-C-0.597300         0    -8.32698   6.78407  -1.45929  L
O-O--0.567900        0    -8.99767   6.26333  -2.34747  L
C-CT-0.365400        0    -7.28377   9.06839  -1.71712  L
O-OH--0.676100       0    -7.50283   10.44113  -1.46861  L
C-CT--0.243800       0    -7.14196   8.91207  -3.23175  L
H-H-0.271900         0    -7.94402   9.13693   0.73206  L
H-H1-0.100700        0    -9.35412   8.6082   -1.66179  L
H-H1-0.004300        0    -6.37064   8.74669  -1.22244  L
H-HC-0.064200        0    -8.08486   9.16045  -3.71938  L
H-HC-0.064200        0    -6.86343   7.88871  -3.48245  L
H-HC-0.064200        0    -6.36895   9.58138  -3.60644  L
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H-HO-0.410200        0    -6.65018   10.8563  -1.27046  L
N-N--0.415700        0    -7.48936   6.10491  -0.68711  L
C-CT--0.058100       -1   -7.36149   4.65901  -0.61063  L
C-C-0.597300         0    -8.71261   3.97151  -0.48498  L
O-O--0.567900        0    -9.03537   3.1417   -1.33558  L
C-CT--0.007400       0    -6.40062   4.35647   0.52936  L
C-CC-0.186800        0    -6.35859   2.9207    0.94534  L
N-NB--0.543200       0    -6.42776   1.82981   0.08546  L
C-CW--0.220700       0    -6.34381   2.48882   2.23394  L
C-CR-0.163500        0    -6.48459   0.75069   0.87394  L
N-NA--0.279500       0    -6.42467   1.12102   2.16258  L
H-H-0.271900         0    -7.00992   6.65312   0.01932  L
H-H1-0.136000        0    -6.92241   4.30011  -1.54043  L
H-HC-0.036700        0    -6.6918    4.93944   1.39774  L
H-HC-0.036700        0    -5.41298   4.67575   0.21039  L
H-H4-0.186200        0    -6.31827   3.10066   3.12703  L
H-H-0.333900         0    -6.47074   0.4769    2.94913  L
H-H5-0.143500        0    -6.57925  -0.26779   0.52228  L
N-N--0.415700        0    -9.50576   4.33716   0.52792  L
C-CT-0.021300        -1   -10.81727   3.74036   0.7286   L
C-C-0.597300         0    -11.7313   3.83137  -0.47144  L
O-O--0.567900        0    -12.35509   2.84791  -0.86759  L
C-CT--0.123100       0    -11.45699   4.11554   2.0826   L
S-SH--0.311900       0    -12.51858   5.58809   2.04608  L
H-H-0.271900         0    -9.18318   5.03382   1.19132  L
H-H1-0.112400        0    -10.61921   2.66972   0.80965  L
H-H1-0.111200        0    -10.67744   4.24859   2.83209  L
H-H1-0.111200        0    -12.0725   3.27493   2.40737  L
H-HS-0.193300        0    -11.59962   6.42215   1.54128  L
N-N--0.415700        0    -11.75872   5.01074  -1.0695   L
C-CT--0.059700       -1   -12.57819   5.27356  -2.22501  L
C-C-0.597300         0    -12.12452   4.55781  -3.49924  L
O-O--0.567900        0    -12.94975   3.95995  -4.18603  L
C-CT-0.130300        0    -12.78064   6.80619  -2.36852  L
C-CT--0.043000       0    -14.10529   7.25985  -1.70493  L
C-CT--0.320400       -1   -12.68718   7.34494  -3.7995   L
C-CT--0.066000       -1   -15.40609   6.89558  -2.45192  L
H-H-0.271900         0    -11.20731   5.75698  -0.65966  L
H-H1-0.086900        0    -13.55594   4.84165  -2.01353  L
H-HC-0.018700        0    -11.97572   7.303    -1.82313  L
H-HC-0.023600        0    -14.07727   8.34456  -1.59213  L
H-HC-0.023600        0    -14.15208   6.83509  -0.70092  L
H-HC-0.088200        0    -11.67365   7.21584  -4.18091  L
H-HC-0.088200        0    -12.91418   8.41109  -3.80769  L
H-HC-0.088200        0    -13.38604   6.82443  -4.4559   L
H-HC-0.018600        0    -16.26199   7.20461  -1.85166  L
H-HC-0.018600        0    -15.46326   5.81979  -2.61721  L
H-HC-0.018600        0    -15.45032   7.41199  -3.41061  L
N-N--0.415700        0    -10.83581   4.61633  -3.82557  L
C-CT--0.024900       -1   -10.25326   3.9516   -4.99643  L
C-C-0.597300         0    -10.43891   2.42158  -4.89483  L
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O-O--0.567900        0    -10.81903   1.79105  -5.87195  L
C-CT-0.211700        0    -8.79617    4.41204  -5.11762  L
O-OH--0.654600       0    -8.37262    4.4136   -6.46403  L
H-H-0.271900         0    -10.22669   5.13749  -3.20274  L
H-H1-0.084300        0    -10.79035   4.28945  -5.88342  L
H-H1-0.035200        0    -8.1504     3.7862   -4.50294  L
H-H1-0.035200        0    -8.71862    5.43909  -4.75908  L
H-HO-0.427500        0    -7.55749    4.92186  -6.53134  L
N-N--0.516300        0    -10.26804   1.8141   -3.70798  L
C-CT-0.038100        -1   -10.61856   0.4027   -3.42971  L
C-C-0.536600         0    -12.10628   0.08178  -3.64896  L
O-O--0.581900        0    -12.44793  -0.81906  -4.41933  L
C-CT--0.030300       0    -10.30285   0.02757  -1.94978  L
C-C-0.799400         0    -9.01678   -0.75811  -1.6961   L
O-O2--0.801400       0    -8.34098   -1.18329  -2.65335  L
O-O2--0.801400       0    -8.64405   -0.95358  -0.52311  L
H-H-0.293600         0    -9.99008    2.39535  -2.92266  L
H-H1-0.088000        0    -10.05594  -0.23858  -4.10203  L
H-HC--0.012200       0    -11.10198  -0.60703  -1.56306  L
H-HC--0.012200       0    -10.30587   0.92447  -1.33207  L
N-N--0.415700        0    -12.97936   0.78063  -2.91092  L
C-CT-0.033700        -1   -14.43531   0.65609  -2.96101  L
C-C-0.597300         0    -14.94463   0.71406  -4.41471  L
O-O--0.567900        0    -15.79681  -0.07643  -4.8149   L
C-CT--0.182500       -1   -15.02337   1.80925  -2.20537  L
H-H-0.271900         0    -12.60208   1.48697  -2.28713  L
H-H1-0.082300        0    -14.74742  -0.28941  -2.51671  L
H-HC-0.060300        0    -14.73341   1.74621  -1.1562   L
H-HC-0.060300        0    -16.11195   1.76534  -2.2622   L
H-HC-0.060300        0    -14.68454   2.7608   -2.61366  L
N-N--0.415700        0    -14.43724   1.69284  -5.17252  L
C-CT--0.025200       -1   -14.7837    1.98455  -6.5575   L
C-C-0.597300         0    -14.31      0.93629  -7.5601   L
O-O--0.567900        0    -15.05883   0.56343  -8.45812  L
H-H-0.271900         0    -13.76109   2.30518  -4.72762  L
H-H1-0.069800        0    -14.3448    2.9412   -6.83816  L
H-H1-0.069800        0    -15.86727   2.06455  -6.64256  L
N-N--0.516300        0    -13.06418   0.48836  -7.41992  L
C-CT-0.039700        -1   -12.45861  -0.5951   -8.19891  L
C-C-0.536600         0    -13.21505  -1.92926  -8.05531  L
O-O--0.581900        0    -13.37284  -2.66014  -9.03006  L
C-CT-0.056000        0    -10.98952  -0.69726  -7.75049  L
C-CT-0.013600        0    -10.13684  -1.78437  -8.40989  L
C-C-0.805400         0    -9.63228   -1.44334  -9.81086  L
O-O2--0.818800       0    -9.68276   -2.3303   -10.69203  L
O-O2--0.818800       0    -9.02074   -0.36521  -9.97395  L
H-H-0.293600         0    -12.48781   0.89797  -6.69178  L
H-H1-0.110500        0    -12.47776  -0.3298   -9.25675  L
H-HC--0.017300       0    -10.9855   -0.88899  -6.67858  L
H-HC--0.017300       0    -10.50319   0.26443  -7.91155  L
H-HC--0.042500       0    -10.69921  -2.71275  -8.41795  L
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H-HC--0.042500       0    -9.253    -1.93908  -7.78983  L
N-N--0.415700        0    -13.66625  -2.25706  -6.83992  L
C-CT--0.025200       -1   -14.39175  -3.49532  -6.5167   L
C-C-0.597300         0    -13.66863  -4.38335  -5.51912  L
O-O--0.567900        0    -14.03669  -5.55147  -5.37549  L
H-H-0.271900         0    -13.52021  -1.56445  -6.11351  L
H-H1-0.069800        0    -14.56493  -4.07828  -7.42172  L
H-H1-0.069800        0    -15.36041  -3.23173  -6.09388  L
N-N--0.415700        0    -12.64353  -3.85798  -4.83207  L
C-CT--0.059700       -1   -11.90925  -4.6096   -3.8135   L
C-C-0.597300         0    -12.91684  -5.13728  -2.78853  L
O-O--0.567900        0    -13.81208  -4.41756  -2.35207  L
C-CT-0.130300        0    -10.76526  -3.77954  -3.17724  L
C-CT--0.043000       0    -9.51026  -3.878    -4.06141  L
C-CT--0.320400       0    -10.33967  -4.2936   -1.78562  L
C-CT--0.066000       0    -9.53927  -3.07202  -5.354    L
H-H-0.271900         0    -12.45904  -2.86802  -4.9521   L
H-H1-0.086900        0    -11.48187  -5.47304  -4.30714  L
H-HC-0.018700        0    -11.0711  -2.73864  -3.0721   L
H-HC-0.023600        0    -9.38226  -4.91516  -4.3289   L
H-HC-0.023600        0    -8.63383  -3.57349  -3.49411  L
H-HC-0.088200        0    -9.51973  -3.68358  -1.40276  L
H-HC-0.088200        0    -10.01484  -5.33289  -1.84634  L
H-HC-0.088200        0    -11.16146  -4.20161  -1.08042  L
H-HC-0.018600        0    -8.60407  -3.22433  -5.89021  L
H-HC-0.018600        0    -9.64493  -2.0159   -5.12943  L
H-HC-0.018600        0    -10.36007  -3.39807  -5.98805  L
N-N--0.415700        0    -12.77113  -6.4108   -2.41723  L
C-CT--0.025200       -1   -13.6354  -7.07525  -1.43361  L
C-C-0.597300         0    -13.0778  -7.05559  -0.02715  L
O-O--0.567900        0    -13.79861  -6.86291   0.94981  L
H-H-0.271900         0    -12.05378  -6.92411  -2.91325  L
H-H1-0.069800        0    -13.78038  -8.11299  -1.72972  L
H-H1-0.069800        0    -14.61445  -6.59371  -1.41848  L
N-N--0.415700        0    -11.77234  -7.27302   0.0562   L
C-CT--0.058100       -1   -11.01448  -7.30546   1.28848  L
C-C-0.597300         0    -9.62327  -6.68746   1.0319   L
O-O--0.567900        0    -8.8993   -7.16689   0.1601   L
C-CT--0.007400       0    -10.89619  -8.76215   1.76975  L
C-CC-0.186800        0    -12.20418  -9.3323    2.27015  L
N-NB--0.543200       0    -12.79865  -9.058     3.50512  L
C-CW--0.220700       0    -13.03621  -10.13688   1.54794  L
C-CR-0.163500        0    -13.98101  -9.68873   3.49158  L
N-NA--0.279500       0    -14.1497  -10.34931   2.33224  L
H-H-0.271900         0    -11.25657  -7.37885  -0.80566  L
H-H1-0.136000        0    -11.51975  -6.72214   2.05986  L
H-HC-0.036700        0    -10.1585  -8.81997   2.56763  L
H-HC-0.036700        0    -10.52762  -9.38241   0.95126  L
H-H4-0.186200        0    -12.85846  -10.48721   0.54139  L
H-H-0.333900         0    -14.97677  -10.86712   2.07477  L
H-H5-0.143500        0    -14.70058  -9.65667   4.29961  L
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N-N--0.415700        0    -9.24807  -5.61158   1.73518  L
C-CT--0.024900       -1   -7.98363  -4.88314   1.50877  L
C-C-0.597300         0    -6.79312  -5.53355   2.21657  L
O-O--0.567900        0    -6.8113   -5.77601   3.42222  L
C-CT-0.211700        0    -8.11441  -3.39863   1.86188  L
O-OH--0.654600       0    -6.84802  -2.7611    1.77379  L
H-H-0.271900         0    -9.85699  -5.31975   2.49207  L
H-H1-0.084300        0    -7.77744  -4.91338   0.43827  L
H-H1-0.035200        0    -8.50879  -3.30035   2.86592  L
H-H1-0.035200        0    -8.814    -2.92209   1.17342  L
H-HO-0.427500        0    -6.87103  -1.98239   2.35767  L
N-N--0.415700        0    -5.72908  -5.79696   1.4572   L
C-CT--0.051800       -1   -4.41826  -6.18552   1.97655  L
C-C-0.597300         0    -3.57469  -4.95154   2.24339  L
O-O--0.567900        0    -3.47269  -4.07938   1.38109  L
C-CT--0.110200       0    -3.7063   -7.1032    0.96093  L
C-CT-0.353100        0    -4.21722  -8.55582   0.88618  L
C-CT--0.412100       0    -5.56001  -8.6996    0.16817  L
C-CT--0.412100       0    -3.19925  -9.40788   0.12134  L
H-H-0.271900         0    -5.82402  -5.61847   0.46911  L
H-H1-0.092200        0    -4.54321  -6.72959   2.91603  L
H-HC-0.045700        0    -2.65884  -7.14749   1.24981  L
H-HC-0.045700        0    -3.74721  -6.65159  -0.02849  L
H-HC--0.036100       0    -4.30642  -8.95693   1.89604  L
H-HC-0.100000        0    -5.51116  -8.24884  -0.82372  L
H-HC-0.100000        0    -6.35142  -8.22246   0.74354  L
H-HC-0.100000        0    -5.81802  -9.75257   0.07206  L
H-HC-0.100000        0    -2.23237  -9.36967   0.62254  L
H-HC-0.100000        0    -3.09584  -9.03604  -0.89809  L
H-HC-0.100000        0    -3.53755  -10.44348   0.08971  L
N-N--0.415700        0    -2.93928  -4.91953   3.40826  L
C-CT-0.021300        -1   -2.0005   -3.87486   3.78772  L
C-C-0.597300         0    -0.86859  -4.43237   4.66854  L
O-O--0.567900        0    -0.88854  -5.60435   5.04835  L
C-CT--0.123100       0    -2.81615  -2.78199   4.48445  L
S-SH--0.311900       0    -1.88453  -1.23509   4.56769  L
H-H-0.271900         0    -3.12769  -5.65002   4.0852   L
H-H1-0.112400        0    -1.5455   -3.44893   2.88958  L
H-H1-0.111200        0    -3.10094  -3.10526   5.4873   L
H-H1-0.111200        0    -3.72127  -2.59506   3.90625  L
H-HS-0.193300        0    -2.78404  -0.57547   5.31146  L
N-N--0.415700        0     0.12616  -3.61872   5.01987  L
C-CT--0.038900       -1    1.23847  -4.03215   5.88921  L
C-C-0.597300         0     1.35315  -3.19694   7.14072  L
O-O--0.567900        0     0.65064  -2.21676   7.36643  L
C-CT-0.365400        0     2.58699  -4.09556   5.14391  L
O-OH--0.676100       0     2.96707  -2.86076   4.57282  L
C-CT--0.243800       0     2.58057  -5.1723    4.06299  L
H-H-0.271900         0     0.04854  -2.64909   4.73645  L
H-H1-0.100700        0     1.04148  -5.04353   6.24489  L
H-H1-0.004300        0     3.36596  -4.38105   5.85092  L
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H-HC-0.064200        0     1.86928  -4.92448   3.27635  L
H-HC-0.064200        0     2.29945  -6.1315    4.49919  L
H-HC-0.064200        0     3.57634  -5.25464   3.63812  L
H-HO-0.410200        0     3.35752  -2.30911   5.2876   L
N-N--0.415700        0     2.22542  -3.68402   8.01106  L
C-CT--0.051800       -1    2.14418  -3.41768   9.42349  L
C-C-0.597300         0     2.24638  -1.9281    9.83254  L
O-O--0.567900        0     1.68211  -1.54846   10.84927  L
C-CT--0.110200       0     3.14376  -4.31177   10.12471  L
C-CT-0.353100        0     2.84389  -4.42379   11.62096  L
C-CT--0.412100       0     1.49433  -5.06133   11.96324  L
C-CT--0.412100       -1    3.92458  -5.34884   12.11659  L
H-H-0.271900         0     2.71571  -4.51351   7.72862  L
H-H1-0.092200        0     1.14018  -3.72387   9.7191   L
H-HC-0.045700        0     4.14394  -3.90272   9.97274  L
H-HC-0.045700        0     3.09601  -5.30961   9.68363  L
H-HC--0.036100       0     2.94692  -3.46037   12.11745  L
H-HC-0.100000        0     1.35952  -6.00047   11.42783  L
H-HC-0.100000        0     0.68275  -4.38169   11.71126  L
H-HC-0.100000        0     1.43223  -5.24253   13.0373  L
H-HC-0.100000        0     3.81853  -5.46576   13.19595  L
H-HC-0.100000        0     4.90831  -4.92297   11.92198  L
H-HC-0.100000        0     3.83945  -6.33126   11.65208  L
N-N--0.516300        0     2.93182  -1.07628   9.06484  L
C-CT-0.039700        -1    3.0897    0.36868   9.34379  L
C-C-0.536600         0     1.86599   1.25032   8.99628  L
O-O--0.581900        0     1.97679   2.4762    8.91895  L
C-CT-0.056000        0     4.3823    0.85408   8.65225  L
C-CT-0.013600        0     4.40816   0.78937   7.11239  L
C-C-0.805400         0     4.95762  -0.51861   6.5309   L
O-O2--0.818800       0     4.27217  -1.56922   6.55621  L
O-O2--0.818800       0     6.12123  -0.52935   6.05199  L
H-H-0.293600         0     3.28023  -1.43101   8.1785   L
H-H1-0.110500        0     3.23058   0.49423   10.41854  L
H-HC--0.017300       0     5.22903   0.28523   9.0405   L
H-HC--0.017300       0     4.54675   1.89173   8.94562  L
H-HC--0.042500       0     5.07524   1.5863    6.78173  L
H-HC--0.042500       0     3.415     0.98604   6.70897  L
N-N--0.415700        0     0.6979    0.62842   8.82679  L
C-CT--0.002400       -1   -0.60841   1.2629    8.61458  L
C-C-0.597300         0    -1.7457    0.65082   9.44681  L
O-O--0.567900        0    -2.91223   1.02008   9.29805  L
C-CT--0.034300       0    -1.00075   1.05064   7.14031  L
C-CA-0.011800        0    -0.0836    1.52259   6.02256  L
C-CA--0.125600       0    -0.29005   2.78856   5.45114  L
C-CA--0.125600       0     0.81786   0.63126   5.40853  L
C-CA--0.170400       0     0.33579   3.13399   4.24127  L
C-CA--0.170400       0     1.47221   0.98471   4.21505  L
C-CA--0.107200       0     1.21467   2.22974   3.61816  L
H-H-0.271900         0     0.73241  -0.38183   8.80506  L
H-H1-0.097800        0    -0.55121   2.32979   8.82834  L
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H-HC-0.029500        0    -1.96721   1.52653   6.97632  L
H-HC-0.029500        0    -1.16266  -0.01881   7.00428  L
H-HA-0.133000        0    -0.97506   3.47444   5.92242  L
H-HA-0.133000        0     0.96522  -0.35234   5.82135  L
H-HA-0.143000        0     0.123     4.09474   3.79736  L
H-HA-0.143000        0     2.13613   0.2809    3.73484  L
H-HA-0.129700        0     1.69832   2.48496   2.68479  L
N-N--0.415700        0    -1.39983  -0.31002   10.29382  L
C-CT--0.003100       -1   -2.27528  -1.19772   11.04147  L
C-C-0.597300         0    -3.50982  -0.49882   11.66968  L
O-O--0.567900        0    -4.6551   -0.80799   11.35697  L
C-CT--0.003600       0    -1.36374  -1.83181   12.11278  L
C-CT--0.064500       0    -2.02995  -2.59563   13.27011  L
C-C-0.695100         0    -1.09637  -2.6802    14.4766  L
O-O--0.608600        0    -0.65002  -3.74356   14.87575  L
N-N--0.940700        0    -0.7615   -1.57681   15.11584  L
H-H-0.271900         0    -0.40439  -0.43915   10.42271  L
H-H1-0.085000        0    -2.65989  -1.97435   10.39381  L
H-HC-0.017100        0    -0.76727  -1.02747   12.54701  L
H-HC-0.017100        0    -0.66975  -2.50817   11.61604  L
H-HC-0.035200        0    -2.29129  -3.59976   12.93508  L
H-HC-0.035200        0    -2.94051  -2.10263   13.60297  L
H-H-0.425100         0    -0.13026  -1.72378   15.87692  L
H-H-0.425100         0    -1.01837  -0.63329   14.81399  L
N-N--0.516300        0    -3.27817   0.39096   12.62876  L
C-CT-0.038100        -1   -4.22935   1.26849   13.34698  L
C-C-0.536600         0    -4.79086   2.36758   12.44176  L
O-O--0.581900        0    -5.97801   2.68477   12.50962  L
C-CT--0.030300       0    -3.48051   1.87318   14.55343  L
C-C-0.799400         0    -2.01139   2.14657   14.20902  L
O-O2--0.801400       0    -1.73673   3.15559   13.52206  L
O-O2--0.801400       0    -1.19405   1.21285   14.40775  L
H-H-0.293600         0    -2.29673   0.51518   12.85406  L
H-H1-0.088000        0    -5.07358   0.68183   13.7102  L
H-HC--0.012200       0    -3.51861   1.15856   15.37762  L
H-HC--0.012200       0    -3.97139   2.79151   14.88008  L
N-N--0.415700        0    -3.93947   2.92452   11.57644  L
C-CT-0.014300        -1   -4.2796    3.96976   10.61509  L
C-C-0.597300         0    -5.52455   3.668     9.78189  L
O-O--0.567900        0    -6.29048   4.57385   9.45344  L
C-CT--0.204100       0    -3.06193   4.32046   9.7399   L
C-C-0.713000         0    -2.11749   5.33655   10.3567  L
O-O--0.593100        0    -1.76336   6.31937   9.72793  L
N-N--0.919100        0    -1.63935   5.16046   11.56644  L
H-H-0.271900         0    -2.98419   2.60228   11.63389  L
H-H1-0.104800        0    -4.54151   4.86459   11.18314  L
H-HC-0.079700        0    -3.42564   4.75532   8.80679  L
H-HC-0.079700        0    -2.49633   3.43346   9.48501  L
H-H-0.419600         0    -1.03138   5.89633   11.86645  L
H-H-0.419600         0    -1.86158   4.38329   12.19275  L
N-N--0.347900        0    -5.74826   2.38829   9.48018  L
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C-CT--0.263700       -1   -6.90738   1.92419   8.7262   L
C-C-0.734100         0    -8.29412   2.25437   9.2941   L
O-O--0.589400        0    -9.28519   2.09877   8.58403  L
C-CT--0.000700       0    -6.76038   0.42558   8.40819  L
C-CT-0.039000        0    -7.3646   -0.47531   9.4893   L
C-CT-0.048600        0    -6.98163  -1.93874   9.28387  L
N-N2--0.529500       0    -7.66053  -2.75533   10.29579  L
C-CA-0.807600        0    -7.15018  -3.17545   11.4275  L
N-N2--0.862700       0    -5.87794  -3.28556   11.64525  L
N-N2--0.862700       0    -7.93586  -3.44052   12.42136  L
H-H-0.274700         0    -5.0412    1.72537   9.78064  L
H-H1-0.156000        0    -6.87242   2.45039   7.77027  L
H-HC-0.032700        0    -5.70261   0.18548   8.28643  L
H-HC-0.032700        0    -7.26976   0.216     7.46602  L
H-HC-0.028500        0    -8.45217  -0.39592   9.46242  L
H-HC-0.028500        0    -7.0164   -0.14974   10.46995  L
H-H1-0.068700        0    -5.9006   -2.02571   9.36567  L
H-H1-0.068700        0    -7.27967  -2.26997   8.29212  L
H-H-0.345600         0    -8.67002  -2.80858   10.2469  L
H-H-0.447800         0    -5.49501  -2.35212   11.74475  L
H-H-0.447800         0    -5.40908  -3.63747   10.80079  L
H-H-0.447800         0    -7.50698  -3.71143   13.28076  L
H-H-0.447800         0    -8.90721  -3.14523   12.33363  L
N-N--0.415700        0    -8.40092   2.68334   10.54827  L
C-CT--0.149000       -1   -9.68086   3.02812   11.14311  L
H-H-0.271900         0    -7.54586   2.77415   11.08641  L
H-H1-0.097600        0    -10.25297   3.66677   10.469   L
H-H1-0.097600        0    -9.51745   3.5534    12.08472  L
H-H1-0.097600        0    -10.24605   2.1142    11.33738  L
C-CT--0.366200       -1   -9.84315   6.29164   9.02432  L
C-C-0.597200         0    -10.57086   5.59217   7.90002  L
O-O--0.567900        0    -11.74475   5.8727    7.69728  L
H-HC-0.112300        0    -9.02254   5.67176   9.38635  L
H-HC-0.112300        0    -10.54283   6.48484   9.8346   L
H-HC-0.112300        0    -9.44771   7.23366   8.64967  L
N-N--0.415700        0    -9.89913   4.67632   7.19811  L
C-CT--0.001400       -1   -10.4453   3.8664    6.08915  L
C-C-0.597300         0    -11.79269   3.19191   6.38438  L
O-O--0.567900        0    -12.67691   3.10203   5.53038  L
C-CT--0.015200       0    -9.33514   2.95507   5.5134   L
C-CA--0.001100       0    -9.76463   1.72281   4.73596  L
C-CA--0.190600       0    -10.38461   0.65327   5.4104   L
C-CA--0.190600       0    -9.48321   1.60999   3.35914  L
C-CA--0.234100       0    -10.77913  -0.49319   4.70159  L
C-CA--0.234100       0    -9.82498   0.43714   2.65627  L
C-C-0.322600         0    -10.48537  -0.60981   3.32882  L
O-OH--0.557900       0    -10.85447  -1.73429   2.67116  L
H-H-0.271900         0    -8.93825   4.51428   7.46     L
H-H1-0.087600        0    -10.68282   4.56952   5.28923  L
H-HC-0.029500        0    -8.68313   2.613     6.30983  L
H-HC-0.029500        0    -8.70609   3.5719    4.87005  L
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H-HA-0.169900        0    -10.56984   0.71943   6.47309  L
H-HA-0.169900        0    -8.98781   2.41671   2.83771  L
H-HA-0.165600        0    -11.29168  -1.29467   5.20404  L
H-HA-0.165600        0    -9.60037   0.32749   1.60265  L
H-HO-0.399200        0    -11.7849  -1.90146   2.90115  L
N-N--0.516300        0    -11.96159   2.74163   7.62     L
C-CT-0.038100        -1   -13.19464   2.17812   8.14588  L
C-C-0.536600         0    -14.38053   3.15327   8.33874  L
O-O--0.581900        0    -15.52306   2.67717   8.39135  L
C-CT--0.030300       0    -12.8682   1.56772   9.53326  L
C-C-0.799400         0    -12.18765   0.19456   9.48583  L
O-O2--0.801400       0    -12.73385  -0.70399   8.80695  L
O-O2--0.801400       0    -11.17212  -0.03873   10.1725  L
H-H-0.293600         0    -11.12715   2.75497   8.19895  L
H-H1-0.088000        0    -13.53168   1.38597   7.47687  L
H-HC--0.012200       0    -13.79612   1.43936   10.09245  L
H-HC--0.012200       0    -12.25676   2.26898   10.10181  L
N-N--0.415700        0    -14.11881   4.45595   8.54424  L
C-CT--0.149000       -1   -15.05072   5.50173   8.99319  L
H-H-0.271900         0    -13.16295   4.74609   8.354    L
H-H1-0.097600        0    -15.95693   5.46789   8.38627  L
H-H1-0.097600        0    -14.58065   6.48016   8.88047  L
H-H1-0.097600        0    -15.31187   5.33996   10.03941  L
C-CT--0.366200       -1   -19.85242  -0.7454   -1.24455  L
C-C-0.597200         0    -18.83764  -0.43415  -0.13348  L
O-O--0.567900        0    -18.42599   0.71482  -0.03396  L
H-HC-0.112300        0    -20.71493  -1.25383  -0.82074  L
H-HC-0.112300        0    -19.37157  -1.36994  -1.99602  L
H-HC-0.112300        0    -20.16531   0.19003  -1.70664  L
N-N--0.415700        0    -18.42242  -1.40474   0.71037  L
C-CT--0.058100       -1   -17.2965  -1.22258   1.67544  L
C-C-0.597300         0    -16.46793  -2.475     1.97713  L
O-O--0.567900        0    -16.9011  -3.30621   2.78001  L
C-CT--0.007400       0    -17.73508  -0.47319   2.94426  L
C-CC-0.186800        0    -16.55733   0.2705    3.52745  L
N-NB--0.543200       0    -15.53093  -0.32402   4.25109  L
C-CW--0.220700       0    -16.21708   1.56891   3.27545  L
C-CR-0.163500        0    -14.5696   0.60668   4.38528  L
N-NA--0.279500       0    -14.97477   1.76805   3.84962  L
H-H-0.271900         0    -18.79683  -2.33175   0.58594  L
H-H1-0.136000        0    -16.62884  -0.51564   1.18902  L
H-HC-0.036700        0    -18.14138  -1.16877   3.67889  L
H-HC-0.036700        0    -18.50711   0.25546   2.69503  L
H-H4-0.186200        0    -16.77771   2.26695   2.66679  L
H-H-0.333900         0    -14.40025   2.60787   3.85078  L
H-H5-0.143500        0    -13.60799   0.45359   4.86254  L
N-N--0.254800        0    -15.27224  -2.61567   1.37296  L
C-CT--0.026600       -1   -14.33046  -3.64917   1.76943  L
C-C-0.589600         0    -13.68375  -3.36129   3.11483  L
O-O--0.574800        0    -13.35927  -2.21578   3.42789  L
C-CT--0.007000       0    -13.245   -3.65816   0.69944  L
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C-CT-0.018900        0    -13.27323  -2.25464   0.09764  L
C-CT-0.019200        0    -14.72545  -1.82068   0.27232  L
H-H1-0.064100        0    -14.82557  -4.62042   1.80124  L
H-HC-0.025300        0    -13.53012  -4.38934  -0.04008  L
H-HC-0.025300        0    -12.26029  -3.90665   1.09878  L
H-HC-0.021300        0    -12.97568  -2.25344  -0.95126  L
H-HC-0.021300        0    -12.62779  -1.5907    0.67186  L
H-H1-0.039100        0    -14.74456  -0.75229   0.48769  L
H-H1-0.039100        0    -15.28255  -2.03377  -0.64146  L
N-N--0.347900        0    -13.36628  -4.40953   3.87663  L
C-CT--0.263700       -1   -12.60507  -4.26349   5.12469  L
C-C-0.734100         0    -11.10139  -4.6299    4.94424  L
O-O--0.589400        0    -10.79276  -5.46951   4.10379  L
C-CT--0.000700       0    -13.3465  -4.91547   6.30471  L
C-CT-0.039000        0    -14.64858  -4.14299   6.63782  L
C-CT-0.048600        0    -14.40406  -2.77793   7.31782  L
N-N2--0.529500       0    -15.32015  -1.71317   6.8462   L
C-CA-0.807600        0    -15.71388  -0.6328    7.50664  L
N-N2--0.862700       0    -15.40768  -0.40659   8.74388  L
N-N2--0.862700       0    -16.38937   0.31157   6.92588  L
H-H-0.274700         0    -13.58031  -5.33093   3.51579  L
H-H1-0.156000        0    -12.55699  -3.20377   5.36289  L
H-HC-0.032700        0    -12.70151  -4.9271    7.18524  L
H-HC-0.032700        0    -13.59336  -5.94578   6.04547  L
H-HC-0.028500        0    -15.2531  -4.75208   7.3105   L
H-HC-0.028500        0    -15.22763  -4.00034   5.72427  L
H-H1-0.068700        0    -13.38552  -2.45055   7.11505  L
H-H1-0.068700        0    -14.49296  -2.90802   8.39785  L
H-H-0.345600         0    -15.51856  -1.68527   5.85089  L
H-H-0.447800         0    -15.62119   0.50743   9.10197  L
H-H-0.447800         0    -14.52217  -0.8469    8.9958   L
H-H-0.447800         0    -16.44558   1.2132    7.38378  L
H-H-0.447800         0    -16.44098   0.25511   5.91531  L
N-N--0.415700        0    -10.16212  -3.94951   5.63296  L
C-CT--0.003100       -1   -8.67825  -4.07066   5.49982  L
C-C-0.597300         0    -8.08356  -4.93599   6.61793  L
O-O--0.567900        0    -8.53065  -4.87442   7.76519  L
C-CT--0.003600       0    -8.02775  -2.67781   5.48117  L
C-CT--0.064500       0    -6.49472  -2.76459   5.36809  L
C-C-0.695100         0    -5.88664  -1.42963   4.99018  L
O-O--0.608600        0    -6.10944  -0.94933   3.89166  L
N-N--0.940700        0    -5.08769  -0.81573   5.83123  L
H-H-0.271900         0    -10.49284  -3.27899   6.31708  L
H-H1-0.085000        0    -8.47133  -4.5642    4.55713  L
H-HC-0.017100        0    -8.29315  -2.13123   6.38454  L
H-HC-0.017100        0    -8.41966  -2.11713   4.63495  L
H-HC-0.035200        0    -6.22352  -3.47676   4.59033  L
H-HC-0.035200        0    -6.07562  -3.10602   6.31227  L
H-H-0.425100         0    -4.80901   0.13561   5.62749  L
H-H-0.425100         0    -4.77451  -1.32023   6.67162  L
N-N--0.415700        0    -7.0424   -5.70109   6.28569  L
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C-CT--0.001400       -1   -6.31313  -6.56508   7.20846  L
C-C-0.597300         0    -4.80897  -6.53789   6.91487  L
O-O--0.567900        0    -4.37317  -6.71028   5.77091  L
C-CT--0.015200       0    -6.8298   -8.01395   7.11651  L
C-CA--0.001100       0    -8.33132  -8.16411   6.95628  L
C-CA--0.190600       0    -9.17523  -8.33559   8.07289  L
C-CA--0.190600       0    -8.88274  -8.08432   5.66473  L
C-CA--0.234100       0    -10.57106  -8.4421    7.89218  L
C-CA--0.234100       0    -10.27095  -8.16759   5.49043  L
C-C-0.322600         0    -11.11956  -8.36203   6.59422  L
O-OH--0.557900       0    -12.45626  -8.47632   6.38493  L
H-H-0.271900         0    -6.75959  -5.71827   5.31019  L
H-H1-0.087600        0    -6.47361  -6.20625   8.22628  L
H-HC-0.029500        0    -6.50607  -8.55628   8.00553  L
H-HC-0.029500        0    -6.36045  -8.49843   6.25857  L
H-HA-0.169900        0    -8.75328  -8.37098   9.06671  L
H-HA-0.169900        0    -8.24296  -7.91634   4.80793  L
H-HA-0.165600        0    -11.23436  -8.57352   8.73237  L
H-HA-0.165600        0    -10.69482  -8.04779   4.51163  L
H-HO-0.399200        0    -12.60209  -8.55566   5.42995  L
N-N--0.516300        0    -4.00104  -6.33742   7.95339  L
C-CT-0.039700        -1   -2.54989  -6.27773   7.82236  L
C-C-0.536600         0    -1.87485  -7.6593    7.86898  L
O-O--0.581900        0    -2.09652  -8.4569    8.77999  L
C-CT-0.056000        0    -1.92214  -5.31669   8.8396   L
C-CT-0.013600        0    -2.17128  -3.8507    8.45244  L
C-C-0.805400         0    -3.64321  -3.4178    8.57047  L
O-O2--0.818800       0    -4.34336  -3.91893   9.48429  L
O-O2--0.818800       0    -4.07908  -2.57264   7.75747  L
H-H-0.293600         0    -4.4061   -6.03405   8.83138  L
H-H1-0.110500        0    -2.3394   -5.86312   6.8425   L
H-HC--0.017300       0    -0.84179  -5.47327   8.83873  L
H-HC--0.017300       0    -2.29097  -5.52432   9.84508  L
H-HC--0.042500       0    -1.8242   -3.69886   7.42858  L
H-HC--0.042500       0    -1.54882  -3.22717   9.09398  L
N-N--0.415700        0    -1.00049  -7.93373   6.89438  L
C-CT--0.002400       -1   -0.26248  -9.19648   6.75593  L
C-C-0.597300         0     1.24485  -8.99251   6.93189  L
O-O--0.567900        0     1.78169  -7.88126   6.98345  L
C-CT--0.034300       0    -0.62136  -9.84165   5.39772  L
C-CA-0.011800        0    -0.03834  -9.14311   4.17677  L
C-CA--0.125600       0    -0.73198  -8.09281   3.54989  L
C-CA--0.125600       0     1.22686  -9.51622   3.68861  L
C-CA--0.170400       0    -0.1296   -7.37279   2.50073  L
C-CA--0.170400       0     1.83307  -8.79641   2.64305  L
C-CA--0.107200       0     1.15542  -7.71732   2.0527   L
H-H-0.271900         0    -0.86377  -7.21687   6.18678  L
H-H1-0.097800        0    -0.59395  -9.8768    7.54127  L
H-HC-0.029500        0    -1.70819  -9.87486   5.30076  L
H-HC-0.029500        0    -0.27519  -10.87552   5.40152  L
H-HA-0.133000        0    -1.70937  -7.80011   3.90964  L
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H-HA-0.133000        0     1.73972  -10.35076   4.13465  L
H-HA-0.143000        0    -0.63755  -6.52557   2.06189  L
H-HA-0.143000        0     2.81881  -9.0659    2.29758  L
H-HA-0.129700        0     1.61629  -7.14116   1.26369  L
N-N--0.415700        0     1.95805  -10.11081   7.04316  L
C-CT--0.024900       -1    3.40266  -10.09343   7.23002  L
C-C-0.597300         0     4.16237  -9.58599   5.98697  L
O-O--0.567900        0     4.03183  -10.12555   4.89038  L
C-CT-0.211700        0     3.92247  -11.48829   7.62281  L
O-OH--0.654600       0     3.66117  -12.48671   6.64219  L
H-H-0.271900         0     1.4616   -10.98207   6.95954  L
H-H1-0.084300        0     3.62352  -9.41918   8.0584   L
H-H1-0.035200        0     3.46263  -11.78626   8.56668  L
H-H1-0.035200        0     5.00066  -11.42574   7.77922  L
H-HO-0.427500        0     2.89612  -12.99627   6.93894  L
N-N--0.347900        0     5.0309   -8.58432   6.15256  L
C-CT--0.263700       -1    5.92857  -8.05452   5.10124  L
C-C-0.734100         0     6.99146  -9.06135   4.62429  L
O-O--0.589400        0     7.04481  -10.20391   5.08486  L
C-CT--0.000700       0     6.52288  -6.73204   5.63315  L
C-CT-0.039000        0     7.6378   -6.89422   6.68141  L
C-CT-0.048600        0     8.00728  -5.57034   7.36665  L
N-N2--0.529500       0     8.34626  -4.48938   6.41443  L
C-CA-0.807600        0     7.60258  -3.44197   6.09908  L
N-N2--0.862700       0     6.3839   -3.32994   6.52964  L
N-N2--0.862700       0     8.05209  -2.46722   5.36817  L
H-H-0.274700         0     5.02976  -8.15288   7.06347  L
H-H1-0.156000        0     5.31086  -7.8175    4.23215  L
H-HC-0.032700        0     5.71255  -6.13676   6.05816  L
H-HC-0.032700        0     6.93061  -6.16326   4.8058   L
H-HC-0.028500        0     8.52833  -7.29578   6.20114  L
H-HC-0.028500        0     7.31744  -7.59782   7.45036  L
H-H1-0.068700        0     8.87039  -5.75075   8.00948  L
H-H1-0.068700        0     7.1841   -5.26591   8.01457  L
H-H-0.345600         0     9.28664  -4.4923    6.02707  L
H-H-0.447800         0     5.85451  -2.47402   6.31643  L
H-H-0.447800         0     5.96247  -4.01133   7.11629  L
H-H-0.447800         0     7.40412  -1.68214   5.27138  L
H-H-0.447800         0     8.9643   -2.46177   4.9368   L
N-N--0.415700        0     7.85895  -8.62218   3.71798  L
C-CT--0.051800       -1    9.19835  -9.16512   3.46287  L
C-C-0.597300         0     10.127   -7.9697    3.678    L
O-O--0.567900        0     10.16033  -7.03849   2.87847  L
C-CT--0.110200       0     9.22913  -9.77125   2.04505  L
C-CT-0.353100        0     10.5637  -10.41821   1.62119  L
C-CT--0.412100       0     10.29554  -11.49627   0.56827  L
C-CT--0.412100       0     11.54049  -9.42705   0.99101  L
H-H-0.271900         0     7.67328  -7.70456   3.31836  L
H-H1-0.092200        0     9.44144  -9.94496   4.18717  L
H-HC-0.045700        0     8.9386   -9.02035   1.30887  L
H-HC-0.045700        0     8.46893  -10.54705   2.02851  L
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H-HC--0.036100       0     11.03039  -10.8886   2.48685  L
H-HC-0.100000        0     11.23563  -11.96007   0.26764  L
H-HC-0.100000        0     9.82381  -11.05143  -0.31     L
H-HC-0.100000        0     9.64789  -12.26985   0.97812  L
H-HC-0.100000        0     12.44075  -9.95278   0.67573  L
H-HC-0.100000        0     11.82353  -8.65609   1.70006  L
H-HC-0.100000        0     11.08262  -8.95612   0.12255  L
N-N--0.415700        0     10.82232  -7.94986   4.8096   L
C-CT-0.014300        -1    12.11898  -7.29775   4.84602  L
C-C-0.597300         0     13.12306  -8.37287   4.34993  L
O-O--0.567900        0     13.07932  -9.48362   4.87997  L
C-CT--0.204100       0     12.49948  -6.87222   6.27489  L
C-C-0.713000         0     11.72887  -5.68525   6.81356  L
O-O--0.593100        0     11.08768  -4.92244   6.10871  L
N-N--0.919100        0     11.76814  -5.48221   8.10901  L
H-H-0.271900         0     10.74629  -8.76595   5.39825  L
H-H1-0.104800        0     12.15379  -6.43586   4.17753  L
H-HC-0.079700        0     13.55566  -6.59829   6.27871  L
H-HC-0.079700        0     12.37397  -7.72027   6.94856  L
H-H-0.419600         0     11.3111  -4.65557   8.44378  L
H-H-0.419600         0     12.34094  -6.07035   8.69226  L
N-N--0.415700        0     13.96789  -8.1102    3.34206  L
C-CT--0.051800       -1    15.05335  -9.0328    2.9552   L
C-C-0.597300         0     16.27193  -8.85398   3.89895  L
O-O--0.567900        0     16.55732  -7.73004   4.30905  L
C-CT--0.110200       0     15.42556  -8.85721   1.4485   L
C-CT-0.353100        0     16.41878  -9.89507   0.84605  L
C-CT--0.412100       0     15.89336  -11.32727   0.99845  L
C-CT--0.412100       -1    16.70019  -9.7027   -0.66451  L
H-H-0.271900         0     13.96792  -7.1955    2.91566  L
H-H1-0.092200        0     14.68466  -10.04858   3.09265  L
H-HC-0.045700        0     15.85265  -7.86474   1.3115   L
H-HC-0.045700        0     14.50944  -8.89394   0.8614   L
H-HC--0.036100       0     17.36616  -9.81903   1.37507  L
H-HC-0.100000        0     14.91202  -11.41832   0.53336  L
H-HC-0.100000        0     15.82787  -11.59994   2.0492   L
H-HC-0.100000        0     16.58362  -12.02211   0.51915  L
H-HC-0.100000        0     15.79752  -9.88908  -1.24233  L
H-HC-0.100000        0     17.48474  -10.38964  -0.982    L
H-HC-0.100000        0     17.04592  -8.68235  -0.83483  L
N-N--0.516300        0     16.98545  -9.93262   4.25924  L
C-CT-0.039700        -1    18.24223  -9.84055   5.04142  L
C-C-0.536600         0     19.33701  -9.03639   4.28135  L
O-O--0.581900        0     19.26668  -8.87877   3.05932  L
C-CT-0.056000        0     18.75292  -11.22569   5.48267  L
C-CT-0.013600        0     18.44485  -11.50166   6.96487  L
C-C-0.805400         0     18.98326  -10.41249   7.91453  L
O-O2--0.818800       0     18.39166  -10.26015   9.00375  L
O-O2--0.818800       0     19.92395  -9.6863    7.50953  L
H-H-0.293600         0     16.72115  -10.83376   3.90221  L
H-H1-0.110500        0     18.01589  -9.24425   5.92589  L
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H-HC--0.017300       0     19.83288  -11.2836   5.33896  L
H-HC--0.017300       0     18.2996  -12.00471   4.86702  L
H-HC--0.042500       0     18.87984  -12.46617   7.23595  L
H-HC--0.042500       0     17.36056  -11.58042   7.07725  L
N-N--0.415700        0     20.31464  -8.44963   4.99032  L
C-CT--0.025200       -1    21.33375  -7.51668   4.44392  L
C-C-0.597300         0     20.73477  -6.22223   3.82255  L
O-O--0.567900        0     21.49156  -5.44797   3.24093  L
H-H-0.271900         0     20.33344  -8.68849   5.98637  L
H-H1-0.069800        0     21.90536  -8.02817   3.66963  L
H-H1-0.069800        0     22.0172  -7.22759   5.24146  L
N-N--0.415700        0     19.41318  -5.95374   3.91318  L
C-CT--0.038900       0     18.6912  -5.01596   3.01066  L
C-C-0.597300         0     17.74418  -4.01398   3.71305  L
O-O--0.567900        0     16.9138  -4.36713   4.54795  L
C-CT-0.365400        0     17.87857  -5.80009   1.95831  L
O-OH--0.676100       0     18.63317  -6.82093   1.34488  L
C-CT--0.243800       0     17.41669  -4.91872   0.7957   L
H-H-0.271900         0     18.84793  -6.61919   4.42497  L
H-H1-0.100700        0     19.4351  -4.43846   2.46328  L
H-H1-0.004300        0     17.00218  -6.23776   2.42957  L
H-HC-0.064200        0     16.76986  -4.11954   1.14863  L
H-HC-0.064200        0     16.85811  -5.52854   0.08537  L
H-HC-0.064200        0     18.28253  -4.49137   0.28928  L
H-HO-0.410200        0     18.85822  -7.49808   2.01103  L
N-N--0.415700        0     17.80889  -2.73256   3.32198  L
C-CT--0.087500       -1    16.91956  -1.62283   3.75478  L
C-C-0.597300         0     15.55183  -1.71901   3.04169  L
O-O--0.567900        0     15.49898  -1.69641   1.81535  L
C-CT-0.298500        0     17.53599  -0.25279   3.37991  L
C-CT--0.319200       -1    16.68855   0.95241   3.87905  L
C-CT--0.319200       -1    18.98472  -0.19029   3.89642  L
H-H-0.271900         0     18.49591  -2.52308   2.61323  L
H-H1-0.096900        0     16.77861  -1.67342   4.83376  L
H-HC--0.029700       0     17.59293  -0.17833   2.29356  L
H-HC-0.079100        0     16.56181   0.90225   4.95959  L
H-HC-0.079100        0     15.71786   0.97098   3.38438  L
H-HC-0.079100        0     17.21912   1.86969   3.62774  L
H-HC-0.079100        0     19.01118  -0.38843   4.96812  L
H-HC-0.079100        0     19.39075   0.80489   3.71231  L
H-HC-0.079100        0     19.62129  -0.90566   3.37632  L
N-N--0.415700        0     14.43175  -1.83089   3.77425  L
C-CT--0.023700       -1    13.11897  -2.2242    3.1975   L
C-C-0.597300         0     11.86801  -1.57997   3.8715   L
O-O--0.567900        0     10.75437  -2.11683   3.8268   L
C-CT-0.034200        0     12.98317  -3.76007   3.37766  L
C-CT-0.001800        0     14.0552  -4.67154   2.75848  L
S-S--0.273700        0     13.55873  -5.52789   1.24054  L
C-CT--0.053600       0     13.65189  -4.15038   0.07231  L
H-H-0.271900         0     14.57379  -1.93753   4.76616  L
H-H1-0.088000        0     13.08136  -1.98619   2.1337   L
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 H-HC-0.024100        0     12.0184  -4.08986   2.98945  L
 H-HC-0.024100        0     12.97936  -3.95944   4.44977  L
 H-H1-0.044000        0     14.30405  -5.43178   3.49819  L
 H-H1-0.044000        0     14.97213  -4.12531   2.5664   L
 H-H1-0.068400        0     14.65211  -3.71675   0.087    L
 H-H1-0.068400        0     12.92415  -3.38602   0.34102  L
 H-H1-0.068400        0     13.43433  -4.5209   -0.92676  L
 N-N--0.415700        0     12.02126  -0.41313   4.50093  L
 C-CT--0.024900       -1    10.91833   0.50631   4.85504  L
 C-C-0.597300         0     10.99906   1.64222   3.8403   L
 O-O--0.567900        0     12.10061   2.15168   3.62414  L
 C-CT-0.211700        0     11.07765   0.97833   6.29743  L
 O-OH--0.654600       0     10.16411   1.99697   6.64234  L
 H-H-0.271900         0     12.93724   0.00363   4.41116  L
 H-H1-0.084300        0     9.95261   0.01061   4.75313  L
 H-H1-0.035200        0     12.08882   1.35396   6.43029  L
 H-H1-0.035200        0     10.93051   0.12714   6.96341  L
 H-HO-0.427500        0     9.27377   1.76264   6.29389  L
 N-N--0.347900        0     9.90583   1.98232   3.13729  L
 C-CT--0.240000       -1    9.9989    2.90396   1.98583  L
 C-C-0.734100         0     10.61409   4.25448   2.42669  L
 O-O--0.589400        0     11.61802   4.65548   1.84285  L
 C-CT--0.009400       0     8.68545   3.06515   1.23214  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.85356   3.52382  -0.22968  H
 C-CT--0.047900       0     7.63976   3.09161  -1.05741  H
 C-CT--0.014300       0     7.47317   3.86115  -2.35361  H
 N-N3--0.385400       0     6.20383   3.44382  -3.03596  H
 H-H-0.274700         0     9.01847   1.5598    3.39091  L
 H-H1-0.142600        0     10.71973   2.4677    1.29247  L
 H-HC-0.036200        0     8.10902   3.82235   1.7546   L
 H-HC-0.036200        0     8.16135   2.10792   1.24823  L
 H-HC-0.010300        0     9.76753   3.09164  -0.64509  H
 H-HC-0.010300        0     8.96863   4.61426  -0.22971  H
 H-HC-0.062100        0     6.71755   3.2531   -0.50217  H
 H-HC-0.062100        0     7.68789   2.01959  -1.27017  H
 H-HP-0.113500        0     8.2967    3.73673  -3.06318  H
 H-HP-0.113500        0     7.38407   4.93559  -2.16291  H
 H-H-0.340000         0     6.38072   2.7962   -3.81599  H
 H-H-0.340000         0     5.78049   4.23709  -3.55301  H
 H-H-0.340000         0     5.4137    2.86685  -2.30357  H
 N-N--0.347900        0     10.14978   4.84518   3.55018  L
 C-CT--0.263700       -1    10.71022   6.03164   4.28478  L
 C-C-0.734100         0     12.03367   5.79319   4.99636  L
 O-O--0.589400        0     12.35889   6.45772   5.97641  L
 C-CT--0.000700       0     9.60009   6.63275   5.17967  L
 C-CT-0.039000        0     8.40327   7.06529   4.30912  L
 C-CT-0.048600        0     7.34499   7.93407   4.99586  L
 N-N2--0.529500       0     6.48139   7.20252   5.94634  L
 C-CA-0.807600        0     5.21852   7.47985   6.23454  L
 N-N2--0.862700       0     4.47298   8.28569   5.54554  L
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N-N2--0.862700       0     4.64836   6.93297   7.26166  L
H-H-0.274700         0     9.31628   4.41213   3.92845  L
H-H1-0.156000        0     10.95723   6.78952   3.53553  L
H-HC-0.032700        0     9.99003   7.51416   5.69157  L
H-HC-0.032700        0     9.27679   5.90301   5.92368  L
H-HC-0.028500        0     7.91703   6.197     3.88019  L
H-HC-0.028500        0     8.7892    7.63622   3.47132  L
H-H1-0.068700        0     6.72964   8.34774   4.20063  L
H-H1-0.068700        0     7.83461   8.76482   5.50663  L
H-H-0.345600         0     6.87797   6.47716   6.52466  L
H-H-0.447800         0     3.52552   8.44764   5.87033  L
H-H-0.447800         0     4.74613   8.64749   4.63868  L
H-H-0.447800         0     3.67182   7.17059   7.43744  L
H-H-0.447800         0     5.0899    6.16753   7.7436   L
N-N--0.347900        0     12.79597   4.83915   4.46551  L
C-CT--0.240000       -1    14.17741   4.50254   4.79423  L
C-C-0.734100         0     15.03259   4.15962   3.54534  L
O-O--0.589400        0     16.25102   4.16709   3.65779  L
C-CT--0.009400       0     14.25974   3.41503   5.89126  L
C-CT-0.018700        0     13.42803   3.81432   7.12436  L
C-CT--0.047900       0     13.55458   2.92505   8.36326  L
C-CT--0.014300       0     12.42397   3.37036   9.3052   L
N-N3--0.385400       0     12.4293   2.64512   10.59799  L
H-H-0.274700         0     12.36954   4.3739    3.67857  L
H-H1-0.142600        0     14.64478   5.40223   5.20105  L
H-HC-0.036200        0     15.30317   3.29777   6.1886   L
H-HC-0.036200        0     13.9051   2.46314   5.49788  L
H-HC-0.010300        0     12.37704   3.81923   6.83412  L
H-HC-0.010300        0     13.71312   4.82442   7.42143  L
H-HC-0.062100        0     14.53228   3.07974   8.82346  L
H-HC-0.062100        0     13.43453   1.87639   8.09231  L
H-HP-0.113500        0     11.46823   3.21352   8.79026  L
H-HP-0.113500        0     12.52518   4.44726   9.47825  L
H-H-0.340000         0     12.30583   1.65337   10.44634  L
H-H-0.340000         0     11.6682   2.97572   11.17949  L
H-H-0.340000         0     13.30016   2.80328   11.0881  L
N-N--0.415700        0     14.43029   3.87681   2.37679  L
C-CT--0.051800       -1    15.06995   3.45888   1.10166  L
C-C-0.597300         0     15.29074   4.58184   0.12498  L
O-O--0.567900        0     16.25229   4.55555  -0.64089  L
C-CT--0.110200       0     14.20036   2.32588   0.51615  L
C-CT-0.353100        0     14.72149   1.67621  -0.78074  L
C-CT--0.412100       0     16.10156   1.04062  -0.60851  L
C-CT--0.412100       0     13.74694   0.57902  -1.21665  L
H-H-0.271900         0     13.42125   3.92029   2.37353  L
H-H1-0.092200        0     16.05441   3.05042   1.33565  L
H-HC-0.045700        0     13.20449   2.72608   0.31919  L
H-HC-0.045700        0     14.10049   1.54523   1.27239  L
H-HC--0.036100       0     14.76724   2.424    -1.57173  L
H-HC-0.100000        0     16.08562   0.31758   0.20604  L
H-HC-0.100000        0     16.84356   1.81051  -0.39892  L
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H-HC-0.100000        0     16.39168   0.5359   -1.52967  L
H-HC-0.100000        0     14.08256   0.14883  -2.16014  L
H-HC-0.100000        0     12.75376   1.00316  -1.35831  L
H-HC-0.100000        0     13.70403  -0.20663  -0.46095  L
N-N--0.415700        0     14.41105   5.57131   0.16072  L
C-CT-0.014300        -1    14.63889   6.78466  -0.5769   L
C-C-0.597300         0     15.73052   7.69182   0.06241  L
O-O--0.567900        0     15.45478   8.79332   0.52971  L
C-CT--0.204100       0     13.28623   7.47503  -0.89167  L
C-C-0.713000         0     12.32584   7.74407   0.26453  L
O-O--0.593100        0     12.63328   7.63694   1.44339  L
N-N--0.919100        0     11.09828   8.09096  -0.05468  L
H-H-0.271900         0     13.65657   5.55344   0.83579  L
H-H1-0.104800        0     15.04844   6.51109  -1.55109  L
H-HC-0.079700        0     12.75382   6.85323  -1.61058  L
H-HC-0.079700        0     13.49131   8.43025  -1.37383  L
H-H-0.419600         0     10.46759   8.39906   0.67834  L
H-H-0.419600         0     10.77699   8.13101  -1.01734  L
N-N--0.415700        0     16.9926   7.22631   0.0269   L
C-CT--0.149000       -1    18.20625   7.88799   0.52551  L
H-H-0.271900         0     17.08493   6.29326  -0.36163  L
H-H1-0.097600        0     18.1725   7.93895   1.61515  L
H-H1-0.097600        0     18.25956   8.9037    0.12888  L
H-H1-0.097600        0     19.09146   7.33095   0.21609  L
C-CT--0.055800       0     4.79979   12.88739   5.05909  L
C-CT-0.000000        0     4.55457   12.57426   3.58073  L
O-OS--0.354800       0     5.7953    12.5292   2.8785   L
C-CT--0.202200       0     3.89882   11.20559   3.40989  L
O-OS--0.524600       0     3.09613   11.19499   2.21869  L
C-CT--0.067000       0     5.13355   10.32992   3.32974  L
O-OH--0.613900       0     4.75317   9.0995    2.76223  L
C-CT--0.006600       0     6.06455   11.18489   2.48635  L
N-N*--0.048400       0     7.4979    10.80922   2.66792  L
C-C-0.753800         0     8.13191   10.01024   1.7042   L
O-O--0.625200        0     7.54927   9.66261   0.67948  L
N-NC--0.758400       0     9.41866   9.60303   1.88824  L
C-CA-0.818500        0     10.06215   10.00168   2.96562  L
N-N2--0.953000       0     11.28005   9.55989   3.1212   L
C-CM--0.521500       0     9.47318   10.80861   3.975    L
C-CM--0.005300       0     8.18741   11.19975   3.7894   L
H-H1-0.067900        0     3.84528   12.91075   5.58646  L
H-H1-0.067900        0     5.44001   12.1294   5.50679  L
H-H1-0.117400        0     3.89628   13.3478   3.18749  L
H-H1-0.061500        0     3.29559   10.95953   4.28648  L
H-H1-0.097200        0     5.56257   10.21962   4.32516  L
H-HO-0.418600        0     3.87199   9.28227   2.37708  L
H-H2-0.202900        0     5.76624   11.05212   1.45314  L
H-H-0.423400         0     11.68468   8.98729   2.38714  L
H-H-0.423400         0     11.82728   9.87295   3.89649  L
H-HA-0.192800        0     10.0117   11.12879   4.85126  L
H-H4-0.195800        0     7.69137   11.83255   4.51649  L
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 P-P-1.166200         0     1.64519   10.44255   2.12955  L
 O-O2--0.776000       0     0.84468   11.05198   1.05586  L
 O-O2--0.776000       0     1.08193   10.23748   3.47858  L
 O-OS--0.498900       0     2.08814   9.00841   1.60123  L
 C-CT-0.055800        0     2.44114   8.81581   0.2493   L    H-H1
1581  0.        0.
 C-CT-0.106500        0     2.46047   7.32857  -0.08912  H
 O-OS--0.354800       0     3.28536   6.66301   0.86146  H
 C-CT-0.202200        0     1.09873   6.61259  -0.13654  H
 O-OH--0.654100       0     0.73356   6.19764  -1.43441  H
 C-CT-0.067000        0     1.31645   5.32784   0.71887  H
 O-OH--0.613900       0     1.52944   4.19164  -0.08911  H
 C-CT-0.039400        0     2.62458   5.58139   1.48693  H
 N-N*--0.025100       0     2.41598   5.83102   2.90173  H
 C-CK-0.200600        0     1.52548   6.67757   3.54753  H
 N-NB--0.607300       0     1.46133   6.48817   4.83959  H
 C-CB-0.051500        0     2.34497   5.45241   5.07517  H
 C-CA-0.700900        0     2.67793   4.70378   6.22544  H
 N-N2--0.901900       0     2.16968   4.96603   7.46266  H
 N-NC--0.761500       0     3.62345   3.75827   6.12515  H
 C-CQ-0.587500        0     4.06649   3.4366    4.90707  H
 N-NC--0.699700       0     3.81889   4.03909   3.7542   H
 C-CB-0.305300        0     2.95124   5.04084   3.89193  H
 H-H1-0.067900        0     3.43181   9.2333    0.08388  L
 H-H1-0.067900        0     1.72228   9.30655  -0.41059  L
 H-H1-0.117400        0     2.89586   7.23444  -1.0869   H
 H-H1-0.061500        0     0.30554   7.22338   0.31603  H
 H-HO-0.437600        0     0.47169   6.94464  -2.01552  H
 H-H1-0.097200        0     0.4883    5.18636   1.41498  H
 H-HO-0.418600        0     5.81648   3.98553   1.30091  H
 H-H2-0.200700        0     3.23896   4.68022   1.39151  H
 H-H5-0.155300        0     0.95794   7.42379   2.99913  H
 H-H-0.411500         0     2.14477   4.1393    8.07078  H
 H-H-0.411500         0     1.28374   5.46123   7.47473  H
 H-H5-0.047300        0     4.76433   2.60845   4.85634  H
 N-N3-0.149300        0    -1.27135   4.40006  -0.37343  H
 C-CT-0.053600        0    -0.70785   3.29855   0.42784  H
 C-CT-0.065100        0    -1.48523   1.9899    0.275    H
 C-CT--0.090300       0    -1.14534   0.99601   1.39252  H
 C-C-0.735400         0    -2.00922  -0.25388   1.33128  H
 O-O--0.613300        0    -1.58481  -1.33585   0.96843  H
 N-N--1.003100        0    -3.33015  -0.03129   1.63297  H
 C-C-0.612300         0     0.73765   3.0787   -0.0192   H
 O-O--0.571300        0     1.15915   2.01645  -0.36412  H
 O-OS--0.421200       0     3.64894   2.63481   0.63021  H
 P-P-1.166200         0     4.33773   1.62681  -0.21667  H
 O-O2--0.776000       0     5.71176   1.17333   0.49753  H
 O-O2--0.776000       0     4.68906   1.9838   -1.69447  H
 O-OS--0.498900       0     3.65571   0.17678  -0.31048  H
 C-CT-0.055800        0     2.95539  -0.27999  -1.46757  H
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 C-CT-0.106500        0     2.36531  -1.67841  -1.17748  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.35513  -2.6493   -0.81837  L
 C-CT-0.039400        0     3.23156  -2.958     0.5709   L
 N-N*--0.025100       0     4.57369  -2.99337   1.20625  L
 C-CB-0.305300        0     5.27214  -4.13671   1.51606  L
 N-NC--0.699700       0     4.86107  -5.42396   1.33898  L
 C-CQ-0.587500        0     5.7611   -6.29862   1.76035  L
 N-NC--0.761500       0     6.95449  -6.06582   2.29262  L
 C-CA-0.700900        0     7.33306  -4.79115   2.40418  L
 N-N2--0.901900       0     8.56441  -4.64618   2.85961  L
 C-CB-0.051500        0     6.47406  -3.72976   2.03157  L
 N-NB--0.607300       0     6.56798  -2.333     2.04985  L
 C-CK-0.200600        0     5.40364  -1.95757   1.57268  L
 C-CT-0.067000        0     2.23118  -1.9744    1.18627  L
 O-OH--0.613900       0     1.51091  -2.52973   2.27847  L
 C-CT-0.202200        0     1.34937  -1.69389  -0.03842  L
 O-OH--0.654100       0     0.41266  -2.7467   -0.26553  L
 H-H-0.199600         0    -2.35424   3.85636  -1.61672  H
 H-H-0.199600         0    -0.56406   4.93344  -0.87749  H
 H-H-0.199600         0    -1.7888    5.04834   0.21463  H
 H-HP-0.101500        0    -0.70636   3.56855   1.49607  H
 H-HC-0.005000        0    -1.23547   1.55738  -0.69563  H
 H-HC-0.005000        0    -2.55663   2.20534   0.26483  H
 H-HC-0.033100        0    -1.29303   1.47481   2.36999  H
 H-HC-0.033100        0    -0.10425   0.68727   1.32857  H
 H-H-0.442900         0    -3.90024  -0.83184   1.86147  H
 H-H-0.442900         0    -3.55108   0.80754   2.169    H
 H-H1-0.067900        0     3.64785  -0.35896  -2.31424  H
 H-H1-0.067900        0     2.14391   0.4012   -1.73321  H
 H-H1-0.117400        0     1.85244  -1.993    -2.0855   L
 H-H2-0.200700        0     2.77682  -3.94475   0.66896  L
 H-H5-0.047300        0     5.48311  -7.33753   1.65778  L
 H-H-0.411500         0     8.95656  -3.7205    2.91764  L
 H-H-0.411500         0     9.13069  -5.48629   2.92089  L
 H-H5-0.155300        0     5.11895  -0.92251   1.44753  L
 H-H1-0.097200        0     2.72366  -1.05163   1.49129  L
 H-HO-0.418600        0     2.08463  -2.58656   3.06688  L
 H-H1-0.061500        0     0.84292  -0.73336   0.03737  L
 H-HO-0.437600        0    -0.36525  -2.48759   0.27431  L
 O-OW--0.834000       0    -10.3533  -2.15014   11.56033  L
 H-HW-0.417000        0    -10.64184  -1.29491   11.16138  L
 H-HW-0.417000        0    -10.65909  -2.79583   10.89941  L
 O-OW--0.834000       0    -10.34869  -3.92368   9.48664  L
 H-HW-0.417000        0    -10.60767  -3.26382   8.81483  L
 H-HW-0.417000        0    -9.72225  -4.48165   8.98723  L
 O-OW--0.834000       0    -10.78269  -1.96183   7.70771  L
 H-HW-0.417000        0    -11.57596  -1.54402   8.12951  L
 H-HW-0.417000        0    -10.12807  -1.2621    7.80656  L
 O-OW--0.834000       0     5.81604   3.33233   2.0291   H
 H-HW-0.417000        0     4.86016   3.31716   2.25539  H
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H-HW-0.417000        0     5.90074   1.89454   1.14648  H
O-OW--0.834000       0     6.90809   4.0027    4.44684  H
H-HW-0.417000        0     6.69206   3.61941   3.57013  H
H-HW-0.417000        0     6.38892   4.8232    4.33527  H
O-OW--0.834000       0     6.29587   2.20636  -5.56448  L
H-HW-0.417000        0     7.18009   1.99416  -5.92002  L
H-HW-0.417000        0     6.0624    3.02405  -6.02359  L
O-OW--0.834000       0     6.23212   4.47304   7.13245  L
H-HW-0.417000        0     5.33711   4.08647   7.12407  L
H-HW-0.417000        0     6.59722   4.17326   6.28566  L
O-OW--0.834000       0     7.80582   1.39597   5.42483  H
H-HW-0.417000        0     7.20682   2.1523    5.30713  H
H-HW-0.417000        0     7.15595   0.67315   5.64728  H
O-OW--0.834000       0     5.64359   6.39309   2.5319   H
H-HW-0.417000        0     5.21162   7.27382   2.5542   H
H-HW-0.417000        0     5.19698   6.01688   1.75347  H
O-OW--0.834000       0     7.54724   14.38216   3.98133  L
H-HW-0.417000        0     6.90185   13.78294   3.57647  L
H-HW-0.417000        0     7.25083   15.25108   3.71022  L
O-OW--0.834000       0    -4.40661   2.18563   5.93013  L
H-HW-0.417000        0    -4.30032   2.0573    6.87735  L
H-HW-0.417000        0    -4.83722   3.08237   5.89392  L
O-OW--0.834000       0     0.33383   1.66444   12.24051  L
H-HW-0.417000        0    -0.03406   1.34526   13.0862  L
H-HW-0.417000        0     0.0111    2.57045   12.2338  L
O-OW--0.834000       0    -1.69605   9.62695   5.94728  L
H-HW-0.417000        0    -1.83245   8.83989   6.52145  L
H-HW-0.417000        0    -1.23496   9.26557   5.18406  L
O-OW--0.834000       0     2.05048   8.19287   6.99356  L
H-HW-0.417000        0     1.55584   7.6528    6.35154  L
H-HW-0.417000        0     1.6496    9.08086   6.86267  L
O-OW--0.834000       0    -4.50776   9.14522   5.62778  L
H-HW-0.417000        0    -4.5727    8.25991   6.04631  L
H-HW-0.417000        0    -3.62206   9.44232   5.88114  L
O-OW--0.834000       0    -2.32077   7.40961   7.30389  L
H-HW-0.417000        0    -3.18997   7.01114   7.06186  L
H-HW-0.417000        0    -2.1609    7.05784   8.19897  L
O-OW--0.834000       0     0.99767   10.4721   6.06255  L
H-HW-0.417000        0     1.09429   10.47176   5.07768  L
H-HW-0.417000        0     0.03831   10.55178   6.17121  L
N-N                  0     6.06087   7.3008   -0.36099  H
H-H                  0     6.47069   7.23268   0.56485  H
H-H                  0     6.04265   8.18735  -0.83653  H
```

**PC**

| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.366200 | -1 | -12.61968 | -11.62444 | -5.5256 | L |
| C-C-0.597200 | 0 | -11.93049 | -10.61338 | -6.41259 | L |
| O-O--0.567900 | 0 | -11.53735 | -10.96787 | -7.51495 | L |
| H-HC-0.112300 | 0 | -12.01996 | -11.77911 | -4.63155 | L |
| H-HC-0.112300 | 0 | -12.70675 | -12.56257 | -6.07168 | L |
| H-HC-0.112300 | 0 | -13.61081 | -11.25695 | -5.26907 | L |
| N-N--0.415700 | 0 | -11.75356 | -9.38868 | -5.9074 | L |
| C-CT--0.058100 | -1 | -10.88593 | -8.3645 | -6.50888 | L |
| C-C-0.597300 | 0 | -9.85915 | -7.84977 | -5.49434 | L |
| O-O--0.567900 | 0 | -10.13588 | -7.77218 | -4.29084 | L |
| C-CT--0.007400 | 0 | -11.68689 | -7.25915 | -7.19286 | L |
| C-CC-0.186800 | 0 | -11.08444 | -6.77384 | -8.48598 | L |
| N-NB--0.543200 | 0 | -11.49383 | -7.16224 | -9.76104 | L |
| C-CW--0.220700 | 0 | -10.20119 | -5.74293 | -8.59644 | L |
| C-CR-0.163500 | 0 | -10.89994 | -6.30797 | -10.6074 | L |
| N-NA--0.279500 | 0 | -10.12117 | -5.44346 | -9.93797 | L |
| H-H-0.271900 | 0 | -12.13105 | -9.18337 | -4.99844 | L |
| H-H1-0.136000 | 0 | -10.31894 | -8.85723 | -7.30063 | L |
| H-HC-0.036700 | 0 | -11.74626 | -6.41216 | -6.51932 | L |
| H-HC-0.036700 | 0 | -12.69804 | -7.60874 | -7.40609 | L |
| H-H4-0.186200 | 0 | -9.76272 | -5.18164 | -7.78687 | L |
| H-H-0.333900 | 0 | -9.75911 | -4.56806 | -10.33593 | L |
| H-H5-0.143500 | 0 | -11.0847 | -6.26788 | -11.6715 | L |
| N-N--0.415700 | 0 | -8.66451 | -7.52113 | -5.98029 | L |
| C-CT--0.038900 | -1 | -7.50767 | -7.01752 | -5.21844 | L |
| C-C-0.597300 | 0 | -6.72898 | -5.94167 | -6.01129 | L |
| O-O--0.567900 | 0 | -7.07851 | -5.62468 | -7.1478 | L |
| C-CT-0.365400 | 0 | -6.52225 | -8.14936 | -4.85826 | L |
| O-OH--0.676100 | 0 | -6.23694 | -8.93098 | -5.97912 | L |
| C-CT--0.243800 | -1 | -7.03932 | -9.09107 | -3.7895 | L |
| H-H-0.271900 | 0 | -8.50856 | -7.72348 | -6.96204 | L |
| H-H1-0.100700 | 0 | -7.84247 | -6.57911 | -4.28559 | L |
| H-H1-0.004300 | 0 | -5.59224 | -7.72087 | -4.48475 | L |
| H-HC-0.064200 | 0 | -7.31579 | -8.52437 | -2.90034 | L |
| H-HC-0.064200 | 0 | -6.26289 | -9.80788 | -3.52664 | L |
| H-HC-0.064200 | 0 | -7.91468 | -9.62586 | -4.15911 | L |
| H-HO-0.410200 | 0 | -5.52987 | -9.56182 | -5.767 | L |
| N-N--0.347900 | 0 | -5.64754 | -5.3716 | -5.44273 | L |
| C-CT--0.263700 | -1 | -4.66494 | -4.51927 | -6.16037 | L |
| C-C-0.734100 | 0 | -3.26551 | -4.56858 | -5.55669 | L |
| O-O--0.589400 | 0 | -3.14807 | -4.76371 | -4.35149 | L |
| C-CT--0.000700 | 0 | -5.18408 | -3.06616 | -6.2766 | L |
| C-CT-0.039000 | 0 | -5.01027 | -2.11729 | -5.06967 | L |
| C-CT-0.048600 | 0 | -5.78292 | -2.4413 | -3.78681 | L |
| N-N2--0.529500 | 0 | -5.15795 | -3.49075 | -2.97429 | L |
| C-CA-0.807600 | 0 | -5.10302 | -3.56284 | -1.66295 | L |
| N-N2--0.862700 | 0 | -5.75818 | -2.77715 | -0.86219 | L |
| N-N2--0.862700 | 0 | -4.34318 | -4.46751 | -1.13134 | L |
| H-H-0.274700 | 0 | -5.41102 | -5.68484 | -4.51344 | L |
| H-H1-0.156000 | 0 | -4.59779 | -4.92955 | -7.16377 | L |

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 H-HC-0.032700        0    -6.23805  -3.0821   -6.55768  L
 H-HC-0.032700        0    -4.65548  -2.6042   -7.11201  L
 H-HC-0.028500        0    -5.38075  -1.14515  -5.38614  L
 H-HC-0.028500        0    -3.95327  -1.99351  -4.83778  L
 H-H1-0.068700        0    -6.80396  -2.71325  -4.04612  L
 H-H1-0.068700        0    -5.80329  -1.52627  -3.19434  L
 H-H-0.345600         0    -4.52454  -4.11451  -3.45104  L
 H-H-0.447800         0    -5.77704  -2.9024    0.13835  L
 H-H-0.447800         0    -6.46665  -2.14208  -1.2536   L
 H-H-0.447800         0    -4.04822  -4.33346  -0.17087  L
 H-H-0.447800         0    -3.91387  -5.17511  -1.72014  L
 N-N--0.415700        0    -2.21058  -4.29341  -6.31693  L
 C-CT--0.002400      -1    -0.96949  -3.76629  -5.72626  L
 C-C-0.597300         0    -1.0444   -2.23489  -5.709    L
 O-O--0.567900        0    -1.17189  -1.64372  -6.78182  L
 C-CT--0.034300       0     0.25542  -4.25944  -6.50314  L
 C-CA-0.011800        0     1.55938  -3.66757  -5.99449  L
 C-CA--0.125600       0     1.99114  -3.90698  -4.67359  L
 C-CA--0.125600       0     2.33542  -2.85316  -6.83928  L
 C-CA--0.170400       0     3.17415  -3.30902  -4.2      L
 C-CA--0.170400       0     3.51996  -2.26504  -6.36849  L
 C-CA--0.107200       0     3.92566  -2.47031  -5.04155  L
 H-H-0.271900         0    -2.39737  -4.15877  -7.30689  L
 H-H1-0.097800        0    -0.86174  -4.13962  -4.71004  L
 H-HC-0.029500        0     0.13025  -4.00724  -7.55767  L
 H-HC-0.029500        0     0.31092  -5.34542  -6.41974  L
 H-HA-0.133000        0     1.40953  -4.5363   -4.01513  L
 H-HA-0.133000        0     2.01839  -2.66458  -7.85236  L
 H-HA-0.143000        0     3.50298  -3.48053  -3.1862   L
 H-HA-0.143000        0     4.10938  -1.64257  -7.02468  L
 H-HA-0.129700        0     4.81432  -1.97569  -4.67732  L
 N-N--0.254800        0    -1.01071  -1.5926   -4.52842  L
 C-CT--0.026600       0    -0.79295  -0.15987  -4.40852  L    H-H2
84    0.        0.
 C-C-0.589600         0     0.72634   0.14507  -4.31224  H
 O-O--0.574800        0     1.36604  -0.01283  -3.28347  H
 C-CT--0.007000       0    -1.53176   0.21923  -3.12828  L
 C-CT-0.018900        0    -1.38226  -1.00672  -2.23322  L
 C-CT-0.019200        0    -1.28017  -2.17246  -3.21569  L
 H-H1-0.064100        0    -1.24787   0.38167  -5.23425  L
 H-HC-0.025300        0    -2.58556   0.37541  -3.35575  L
 H-HC-0.025300        0    -1.09975   1.10349  -2.66821  L
 H-HC-0.021300        0    -2.23853  -1.11889  -1.56736  L
 H-HC-0.021300        0    -0.46163  -0.92472  -1.66048  L
 H-H1-0.039100        0    -0.47671  -2.84387  -2.91021  L
 H-H1-0.039100        0    -2.23054  -2.7037   -3.23356  L
 N-N--0.254800        0     1.36662   0.58982  -5.43263  H
 C-CT--0.026600       0     2.62061   1.28444  -5.25894  H
 C-C-0.589600         0     2.31704   2.68055  -4.68966  H
 O-O--0.574800        0     1.17155   3.11148  -4.63844  H
 C-CT--0.007000       0     3.11578   1.45836  -6.69981  H
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 C-CT-0.018900        0     1.81956   1.80632  -7.43524  H
 C-CT-0.019200        0     0.73773   1.00178  -6.69259  H
 H-H1-0.064100        0     3.30757   0.73694  -4.6109   H
 H-HC-0.025300        0     3.53952   0.5199   -7.0561   H
 H-HC-0.025300        0     3.87434   2.23784  -6.79184  H
 H-HC-0.021300        0     1.84817   1.56553  -8.4987   H
 H-HC-0.021300        0     1.62214   2.87576  -7.33433  H
 H-H1-0.039100        0    -0.13952   1.6236   -6.49989  H
 H-H1-0.039100        0     0.44828   0.12105  -7.26914  H
 N-N--0.415700        0     3.41638   3.37743  -4.34536  H
 C-CT-0.039700        0     3.4528    4.82051  -4.18984  H
 C-C-0.597300         0     4.38237   5.33395  -5.32916  L    H-H1
111   0.        0.
 O-O--0.567900        0     5.54218   4.92309  -5.37258  L
 C-CT--0.003600       0     3.83248   5.11455  -2.7316   H
 C-CT-0.013600        0     4.30358   6.52285  -2.43736  H
 C-C-0.805400         0     4.87128   6.63243  -1.04139  H
 O-O2--0.818800       0     4.77237   5.75821  -0.17059  H
 H-H-0.271900         0     4.33664   2.97151  -4.47289  H
 H-H1-0.110500        0     2.44587   5.19592  -4.37365  H
 H-HC--0.017300       0     2.95415   4.89095  -2.11722  H
 H-HC--0.017300       0     4.59846   4.4068   -2.40844  H
 H-HC--0.042500       0     3.49458   7.25744  -2.52873  H
 H-HC--0.042500       0     5.09578   6.83812  -3.12639  H
 N-N--0.254800        0     3.89734   6.1051   -6.32771  L
 C-CT--0.026600      -1     4.67046   6.61092  -7.48094  L
 C-C-0.589600         0     6.0896    7.1411   -7.1916   L
 O-O--0.574800        0     6.97561   7.03247  -8.03912  L
 C-CT--0.007000       0     3.74522   7.58022  -8.20469  L
 C-CT-0.018900        0     2.40167   6.88928  -7.99912  L
 C-CT-0.019200        0     2.49262   6.42173  -6.5467   L
 H-H1-0.064100        0     4.80569   5.76449  -8.14974  L
 H-HC-0.025300        0     3.99704   7.68616  -9.26032  L
 H-HC-0.025300        0     3.73971   8.53593  -7.69644  L
 H-HC-0.021300        0     2.33259   6.02597  -8.65877  L
 H-HC-0.021300        0     1.56025   7.55309  -8.1705   L
 H-H1-0.039100        0     2.19433   7.22369  -5.87095  L
 H-H1-0.039100        0     1.85663   5.54823  -6.40699  L
 N-N--0.415700        0     6.36146   7.63356  -5.9831   L
 C-CT-0.014300       -1     7.70307   7.82307  -5.44161  L
 C-C-0.597300         0     8.50885   6.53646  -5.36267  L
 O-O--0.567900        0     8.33172   5.71843  -4.4613   L
 C-CT--0.204100       0     7.60853   8.48317  -4.04936  L
 C-C-0.713000         0     8.96611   8.87369  -3.48751  L
 O-O--0.593100        0     9.50078   8.26542  -2.57042  L
 N-N--0.919100        0     9.56891   9.91753  -4.00088  L
 H-H-0.271900         0     5.54957   7.83171  -5.39891  L
 H-H1-0.104800        0     8.22613   8.51485  -6.10449  L
 H-HC-0.079700        0     7.13749   7.79408  -3.35317  L
 H-HC-0.079700        0     6.99366   9.37311  -4.10831  L
 H-H-0.419600         0     10.45953   10.16319  -3.61435  L
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H-H-0.419600         0     9.12237   10.49159  -4.71646  L
N-N--0.415700        0     9.50209   6.43406  -6.22976  L
C-CT--0.025200       -1    10.68987   5.6702   -5.92147  L
C-C-0.597300         0     11.04576   4.66453  -7.0214   L
O-O--0.567900        0     11.55564   5.01893  -8.07876  L
H-H-0.271900         0     9.5038    7.05107  -7.03063  L
H-H1-0.069800        0     10.59371   5.14451  -4.97122  L
H-H1-0.069800        0     11.52754   6.36115  -5.82908  L
N-N--0.415700        0     10.78874   3.39868  -6.71795  L
C-CT--0.001400       -1    10.81535   2.19475  -7.56025  L
C-C-0.597300         0     9.76143   1.27203  -6.92524  L
O-O--0.567900        0     8.94946   1.72201  -6.10531  L
C-CT--0.015200       0     12.24867   1.61807  -7.56889  L
C-CA--0.001100       0     12.74494   1.22454  -8.94581  L
C-CA--0.190600       0     13.16889   2.23101  -9.83597  L
C-CA--0.190600       0     12.80774  -0.12845  -9.33301  L
C-CA--0.234100       0     13.6637   1.8901   -11.1096  L
C-CA--0.234100       0     13.29284  -0.47286  -10.60944  L
C-C-0.322600         0     13.72424   0.53382  -11.49755  L
O-OH--0.557900       0     14.18732   0.1957   -12.7289  L
H-H-0.271900         0     10.28794   3.26702  -5.8511   L
H-H1-0.087600        0     10.50458   2.44715  -8.57581  L
H-HC-0.029500        0     12.32573   0.76876  -6.88924  L
H-HC-0.029500        0     12.94342   2.36948  -7.18936  L
H-HA-0.169900        0     13.10998   3.27034  -9.53548  L
H-HA-0.169900        0     12.49123  -0.90968  -8.65685  L
H-HA-0.165600        0     13.98628   2.66682  -11.78504  L
H-HA-0.165600        0     13.3416  -1.50486  -10.92198  L
H-HO-0.399200        0     14.46269   0.96814  -13.22256  L
N-N--0.415700        0     9.83078  -0.02436  -7.16955  L
C-CT--0.051800       -1    9.38238  -1.01816  -6.19906  L
C-C-0.597300         0     10.53782  -1.95759  -5.89566  L
O-O--0.567900        0     11.51612  -2.05227  -6.63604  L
C-CT--0.110200       0     8.0877   -1.69066  -6.70766  L
C-CT-0.353100        0     8.1389   -2.37656  -8.09029  L
C-CT--0.412100       0     8.71796  -3.7924   -8.01642  L
C-CT--0.412100       0     6.71917  -2.48315  -8.64867  L
H-H-0.271900         0     10.4532  -0.32835  -7.9074   L
H-H1-0.092200        0     9.15014  -0.51191  -5.26542  L
H-HC-0.045700        0     7.33148  -0.90473  -6.74547  L
H-HC-0.045700        0     7.74522  -2.41812  -5.97276  L
H-HC--0.036100       0     8.73043  -1.7861   -8.78782  L
H-HC-0.100000        0     9.76748  -3.75608  -7.7343   L
H-HC-0.100000        0     8.64963  -4.262    -8.99791  L
H-HC-0.100000        0     8.16325  -4.39111  -7.29453  L
H-HC-0.100000        0     6.09167  -3.07199  -7.98512  L
H-HC-0.100000        0     6.74047  -2.94446  -9.63715  L
H-HC-0.100000        0     6.28715  -1.48965  -8.74519  L
N-N--0.415700        0     10.45521  -2.59654  -4.74369  L
C-CT--0.058100       -1    11.54378  -3.36724  -4.15801  L
C-C-0.597300         0     11.04185  -4.75695  -3.79103  L
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 O-O--0.567900        0     9.84193  -5.02116  -3.77534  L
 C-CT--0.007400       0     12.09302  -2.59037  -2.94746  L
 C-CC-0.186800        0     11.06051  -2.2677   -1.88847  L
 N-NB--0.543200       0     10.74759  -3.06027  -0.78445  L
 C-CW--0.220700       0     10.24203  -1.17683  -1.89016  L
 C-CR-0.163500        0     9.75878  -2.42162  -0.13639  L
 N-NA--0.279500       0     9.4207   -1.2993   -0.79014  L
 H-H-0.271900         0     9.59082  -2.49819  -4.22518  L
 H-H1-0.136000        0     12.34589  -3.49182  -4.88784  L
 H-HC-0.036700        0     12.52004  -1.65199  -3.30399  L
 H-HC-0.036700        0     12.90197  -3.15904  -2.49404  L
 H-H4-0.186200        0     10.21084  -0.40479  -2.64679  L
 H-H-0.333900         0     8.61796  -0.71984  -0.56942  L
 H-H5-0.143500        0     9.26383  -2.78039   0.75757  L
 N-N--0.415700        0     11.95033  -5.67775  -3.48957  L
 C-CT--0.059700       -1    11.54635  -7.04873  -3.17542  L
 C-C-0.597300         0     10.62472  -7.1659   -1.93536  L
 O-O--0.567900        0     9.85259  -8.11666  -1.82961  L
 C-CT-0.130300        0     12.77464  -7.96896  -3.07186  L
 C-CT--0.043000       0     12.30571  -9.43626  -2.98553  L
 C-CT--0.320400       0     13.69811  -7.59093  -1.89837  L
 C-CT--0.066000       -1    13.3681  -10.42131  -3.45117  L
 H-H-0.271900         0     12.9299  -5.44419  -3.53458  L
 H-H1-0.086900        0     10.96254  -7.40172  -4.02318  L
 H-HC-0.018700        0     13.3409  -7.84951  -3.99773  L
 H-HC-0.023600        0     11.43739  -9.58089  -3.62914  L
 H-HC-0.023600        0     12.018   -9.68097  -1.96212  L
 H-HC-0.088200        0     14.59834  -8.2016   -1.93065  L
 H-HC-0.088200        0     13.19719  -7.75542  -0.9436   L
 H-HC-0.088200        0     14.00379  -6.54805  -1.96608  L
 H-HC-0.018600        0     12.96728  -11.43406  -3.40016  L
 H-HC-0.018600        0     14.24792  -10.36048  -2.81103  L
 H-HC-0.018600        0     13.65238  -10.20564  -4.48172  L
 N-N--0.415700        0     10.6458  -6.19094  -1.01892  L
 C-CT--0.025200       -1    9.61685  -6.04669   0.01247  L
 C-C-0.597300         0     8.22514  -5.92182  -0.60602  L
 O-O--0.567900        0     7.40598  -6.83223  -0.47116  L
 H-H-0.271900         0     11.27898  -5.41696  -1.15475  L
 H-H1-0.069800        0     9.82512  -5.17486   0.62781  L
 H-H1-0.069800        0     9.62559  -6.92907   0.64739  L
 N-N--0.415700        0     7.98287  -4.83516  -1.35134  L
 C-CT--0.058100       0     6.78565  -4.6607   -2.1907   L    H-HC
246   0.        0.
 C-C-0.597300         0     6.43553  -5.93319  -2.97888  L
 O-O--0.567900        0     5.26437  -6.29801  -3.04314  L
 C-CT--0.007400       0     6.96458  -3.50512  -3.18003  H
 C-CC-0.186800        0     6.92292  -2.079    -2.72989  H
 N-NB--0.543200       0     7.4605   -1.16151  -3.59918  H
 C-CW--0.220700       0     6.28569  -1.43097  -1.70442  H
 C-CR-0.163500        0     7.09972   0.01548  -3.1469   H
 N-NA--0.279500       0     6.41002  -0.08514  -1.98311  H
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H-H-0.271900          0     8.74923  -4.18391  -1.46965  L
H-H1-0.136000         0     5.9268   -4.43973  -1.55362  L
H-HC-0.036700         0     6.17879  -3.61981  -3.93531  H
H-HC-0.036700         0     7.89257  -3.6416   -3.72995  H
H-H4-0.186200         0     5.73244  -1.76951  -0.84754  H
H-H-0.333900          0     5.8992    0.68268  -1.55668  H
H-H5-0.143500         0     7.2929    0.97358  -3.61521  H
N-N--0.415700         0     7.42809  -6.63055  -3.54721  L
C-CT-0.033700         -1    7.23373  -7.88527  -4.27633  L
C-C-0.597300          0     6.42279  -8.94783  -3.52983  L
O-O--0.567900         0     5.59294  -9.61274  -4.14929  L
C-CT--0.182500        0     8.54914  -8.4243   -4.84302  L
H-H-0.271900          0     8.35787  -6.22938  -3.49616  L
H-H1-0.082300         0     6.62477  -7.62734  -5.14089  L
H-HC-0.060300         0     9.10077  -7.62136  -5.33312  L
H-HC-0.060300         0     8.32902  -9.19621  -5.58176  L
H-HC-0.060300         0     9.14768  -8.87302  -4.0557   L
N-N--0.347900         0     6.58989  -9.09078  -2.21029  L
C-CT--0.240000        -1    5.69779  -9.94473  -1.41555  L
C-C-0.734100          0     4.22358  -9.48646  -1.47755  L
O-O--0.589400         0     3.3449   -10.32942  -1.63644  L
C-CT--0.009400        0     6.20974  -10.08792   0.02745  L
C-CT-0.018700         0     5.31641  -11.03181   0.85873  L
C-CT--0.047900        0     5.93396  -11.33468   2.22791  L
C-CT--0.014300        0     4.96342  -12.10469   3.13147  L
N-N3--0.385400        0     5.54071  -12.31286   4.48428  L
H-H-0.274700          0     7.27245  -8.48663  -1.75755  L
H-H1-0.142600         0     5.70895  -10.93788  -1.86833  L
H-HC-0.036200         0     6.24226  -9.10802   0.50309  L
H-HC-0.036200         0     7.22353  -10.49052  -0.00493  L
H-HC-0.010300         0     5.1734   -11.96981   0.31979  L
H-HC-0.010300         0     4.34418  -10.56185   1.01096  L
H-HC-0.062100         0     6.1807   -10.38727   2.70559  L
H-HC-0.062100         0     6.84326  -11.92061   2.08599  L
H-HP-0.113500         0     4.70558  -13.0603   2.66598  L
H-HP-0.113500         0     4.04689  -11.51145   3.22233  L
H-H-0.340000          0     4.818    -12.56896   5.15282  L
H-H-0.340000          0     5.9007   -11.4245   4.83379  L
H-H-0.340000          0     6.28776  -12.98913   4.48762  L
N-N--0.415700         0     3.94187  -8.18444  -1.34907  L
C-CT--0.024900        -1    2.59421  -7.6001   -1.52696  L
C-C-0.597300          0     2.04139  -7.86651  -2.93751  L
O-O--0.567900         0     0.91231  -8.33928  -3.03767  L
C-CT-0.211700         0     2.59501  -6.09337  -1.20649  L
O-OH--0.654600        0     1.26419  -5.6302   -1.07017  L
H-H-0.271900          0     4.73381  -7.5564   -1.30706  L
H-H1-0.084300         0     1.92061  -8.08553  -0.82     L
H-H1-0.035200         0     3.09618  -5.53724  -1.99823  L
H-H1-0.035200         0     3.12386  -5.92672  -0.26785  L
H-HO-0.427500         0     1.25089  -4.69575  -0.79119  L
N-N--0.415700         0     2.8204   -7.64569  -4.01402  L
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C-CT--0.059700       -1    2.49096  -8.07256  -5.40104  L
C-C-0.597300         0     2.06804  -9.55951  -5.3742   L
O-O--0.567900        0     0.93877  -9.87226  -5.73087  L
C-CT-0.130300        0     3.64559  -7.80006  -6.39628  L
C-CT--0.043000       0     4.03185  -6.30476  -6.40538  L
C-CT--0.320400       0     3.24945  -8.24288  -7.81725  L
C-CT--0.066000       0     5.26963  -5.97689  -7.24707  L
H-H-0.271900         0     3.72407  -7.21848  -3.83776  L
H-H1-0.086900        0     1.62352  -7.5      -5.73166  L
H-HC-0.018700        0     4.51492  -8.37997  -6.09252  L
H-HC-0.023600        0     4.24271  -5.97644  -5.39039  L
H-HC-0.023600        0     3.193    -5.71905  -6.77847  L
H-HC-0.088200        0     2.42195  -7.63514  -8.18522  L
H-HC-0.088200        0     2.95468  -9.29228  -7.83431  L
H-HC-0.088200        0     4.09346  -8.13204  -8.49746  L
H-HC-0.018600        0     5.02055  -5.99181  -8.30823  L
H-HC-0.018600        0     6.06763  -6.69152  -7.05215  L
H-HC-0.018600        0     5.618    -4.98185  -6.97927  L
N-N--0.415700        0     2.92622  -10.47382  -4.90297  L
C-CT-0.021300        -1    2.69501  -11.93135  -4.90803  L
C-C-0.597300         0     1.46765  -12.42643  -4.14435  L
O-O--0.567900        0     0.90773  -13.45667  -4.50391  L
C-CT--0.123100       -1    4.00002  -12.67576  -4.49205  L
S-SH--0.311900       0     5.34876  -12.34151  -5.66177  L
H-H-0.271900         0     3.83332  -10.14117  -4.59981  L
H-H1-0.112400        0     2.49764  -12.21364  -5.94417  L
H-H1-0.111200        0     3.80051  -13.74937  -4.48826  L
H-H1-0.111200        0     4.2925   -12.36867  -3.48718  L
H-HS-0.193300        0     5.51608  -11.04944  -5.34258  L
N-N--0.415700        0     1.04523  -11.71923  -3.10076  L
C-CT--0.051800       -1   -0.19191  -12.02064  -2.38639  L
C-C-0.597300         0    -1.41777  -11.37022  -3.05368  L
O-O--0.567900        0    -2.39837  -12.06844  -3.2851   L
C-CT--0.110200       0    -0.04535  -11.54914  -0.92839  L
C-CT-0.353100        0     0.96649  -12.38228  -0.11737  L
C-CT--0.412100       0     1.3136   -11.65699   1.1807   L
C-CT--0.412100       0     0.41653  -13.76289   0.24796  L
H-H-0.271900         0     1.59493  -10.9113  -2.83567  L
H-H1-0.092200        0    -0.36979  -13.09679  -2.39523  L
H-HC-0.045700        0    -1.01783  -11.60351  -0.43677  L
H-HC-0.045700        0     0.26736  -10.50317  -0.93205  L
H-HC--0.036100       0     1.88849  -12.51233  -0.68313  L
H-HC-0.100000        0     1.76708  -10.69867   0.93195  L
H-HC-0.100000        0     2.01769  -12.2485   1.76114  L
H-HC-0.100000        0     0.4083   -11.4824   1.76402  L
H-HC-0.100000        0     1.1453   -14.3087   0.84489  L
H-HC-0.100000        0     0.21922  -14.3358  -0.65779  L
H-HC-0.100000        0    -0.51137  -13.66027   0.81149  L
N-N--0.415700        0    -1.3836   -10.06902  -3.38299  L
C-CT-0.014300        -1   -2.48017  -9.37305  -4.0854   L
C-C-0.597300         0    -2.84075  -10.06297  -5.38651  L
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O-O--0.567900        0    -3.99148  -10.45238  -5.58799  L
C-CT--0.204100       0    -2.20214  -7.87036  -4.20638  L
C-C-0.713000         0    -2.41     -7.16896  -2.87281  L
O-O--0.593100        0    -3.51923  -6.85086  -2.46876  L
N-N--0.919100        0    -1.35995  -6.90709  -2.13507  L
H-H-0.271900         0    -0.52491  -9.56053  -3.20727  L
H-H1-0.104800        0    -3.37472  -9.47776  -3.4663   L
H-HC-0.079700        0    -2.91422  -7.442    -4.9102   L
H-HC-0.079700        0    -1.19761  -7.69041  -4.58699  L
H-H-0.419600         0    -1.48669  -6.39728  -1.28168  L
H-H-0.419600         0    -0.44305  -7.20199  -2.44313  L
N-N--0.415700        0    -1.82866  -10.29703  -6.21016  L
C-CT--0.002400       -1   -1.97136  -11.11981  -7.38964  L
C-C-0.597300         0    -2.17309  -12.61204  -7.14084  L
O-O--0.567900        0    -2.66987  -13.31646  -8.01385  L
C-CT--0.034300       0    -0.83114  -10.84326  -8.38502  L
C-CA-0.011800        0    -0.95389  -9.49269  -9.07522  L
C-CA--0.125600       0    -1.68549  -9.38638  -10.27406  L
C-CA--0.125600       0    -0.39609  -8.33236  -8.50353  L
C-CA--0.170400       0    -1.87237  -8.13251  -10.88383  L
C-CA--0.170400       0    -0.57324  -7.07949  -9.11954  L
C-CA--0.107200       0    -1.31973  -6.97772  -10.3054  L
H-H-0.271900         0    -0.90347  -9.964    -5.96525  L
H-H1-0.097800        0    -2.888    -10.80518  -7.89185  L
H-HC-0.029500        0    -0.85171  -11.61276  -9.15821  L
H-HC-0.029500        0     0.1334   -10.92489  -7.88656  L
H-HA-0.133000        0    -2.1352   -10.26443  -10.71533  L
H-HA-0.133000        0     0.14833  -8.39647  -7.57715  L
H-HA-0.143000        0    -2.46602  -8.04866  -11.78481  L
H-HA-0.143000        0    -0.15822  -6.18753  -8.67702  L
H-HA-0.129700        0    -1.4848   -6.01262  -10.76591  L
N-N--0.415700        0    -1.83358  -13.08516  -5.94787  L
C-CT--0.025200       -1   -2.05459  -14.4538  -5.51253  L
C-C-0.597300         0    -3.51683  -14.86082  -5.36783  L
O-O--0.567900        0    -3.87568  -15.99528  -5.66895  L
H-H-0.271900         0    -1.45072  -12.43924  -5.27675  L
H-H1-0.069800        0    -1.56886  -14.60094  -4.54877  L
H-H1-0.069800        0    -1.58907  -15.13053  -6.22952  L
N-N--0.415700        0    -4.34851  -13.94515  -4.87361  L
C-CT--0.059700       -1   -5.80937  -14.09664  -4.81101  L
C-C-0.597300         0    -6.47137  -14.05631  -6.19174  L
O-O--0.567900        0    -7.49294  -14.71    -6.39588  L
C-CT-0.130300        0    -6.36398  -13.04472  -3.79422  L
C-CT--0.043000       0    -6.03996  -13.52883  -2.34061  L
C-CT--0.320400       -1   -7.87797  -12.71541  -3.94997  L
C-CT--0.066000       -1   -5.35648  -12.51936  -1.38815  L
H-H-0.271900         0    -3.93359  -13.0654  -4.59064  L
H-H1-0.086900        0    -6.03802  -15.08959  -4.4218   L
H-HC-0.018700        0    -5.82635  -12.11127  -3.96911  L
H-HC-0.023600        0    -5.38108  -14.39699  -2.38331  L
H-HC-0.023600        0    -6.96135  -13.87211  -1.86842  L
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H-HC-0.088200        0    -8.06071  -12.24187  -4.9167   L
H-HC-0.088200        0    -8.18964  -12.02581  -3.16562  L
H-HC-0.088200        0    -8.46786  -13.63053  -3.88688  L
H-HC-0.018600        0    -4.40247  -12.20235  -1.79979  L
H-HC-0.018600        0    -5.1917   -12.98512  -0.41644  L
H-HC-0.018600        0    -5.99904  -11.6475  -1.26535  L
N-N--0.415700        0    -5.86933  -13.33527  -7.14064  L
C-CT--0.149000       -1   -6.27273  -13.33072  -8.53479  L
H-H-0.271900         0    -5.02325  -12.85356  -6.87997  L
H-H1-0.097600        0    -6.55683  -14.33864  -8.84298  L
H-H1-0.097600        0    -5.44625  -12.98497  -9.15687  L
H-H1-0.097600        0    -7.1295   -12.66536  -8.66281  L
C-CT--0.366200       -1   -8.69248  -10.19345  -10.71262  L
C-C-0.597200         0    -7.94239  -9.50227  -9.64028  L
O-O--0.567900        0    -8.2975   -9.51096  -8.46918  L
H-HC-0.112300        0    -8.05457  -10.92204  -11.20729  L
H-HC-0.112300        0    -9.07224  -9.45687  -11.419   L
H-HC-0.112300        0    -9.54103  -10.70335  -10.25484  L
N-N--0.415700        0    -6.87765  -8.88827  -10.09987  L
C-CT-0.021300        -1   -6.08259  -8.01652  -9.29413  L
C-C-0.597300         0    -5.58233  -6.86469  -10.16492  L
O-O--0.567900        0    -4.97606  -7.12253  -11.20838  L
C-CT--0.123100       0    -4.88552  -8.80607  -8.74247  L
S-SH--0.311900       0    -3.80175  -7.71393  -7.76464  L
H-H-0.271900         0    -6.69002  -8.91286  -11.08926  L
H-H1-0.112400        0    -6.6699   -7.62284  -8.46554  L
H-H1-0.111200        0    -4.31921  -9.22896  -9.57174  L
H-H1-0.111200        0    -5.25138  -9.62413  -8.12164  L
H-HS-0.193300        0    -3.30844  -7.01897  -8.8029   L
N-N--0.415700        0    -5.80019  -5.61678  -9.74691  L
C-CT-0.014300        -1   -5.33376  -4.45589  -10.50078  L
C-C-0.597300         0    -3.95419  -3.9157   -10.02081  L
O-O--0.567900        0    -3.39072  -4.35364  -9.01369  L
C-CT--0.204100       0    -6.45193  -3.39871  -10.59206  L
C-C-0.713000         0    -6.25743  -2.41643  -11.7456  L
O-O--0.593100        0    -5.42742  -2.60804  -12.62444  L
N-N--0.919100        0    -6.96581  -1.32181  -11.77901  L
H-H-0.271900         0    -6.32793  -5.47864  -8.89008  L
H-H1-0.104800        0    -5.16329  -4.78791  -11.52669  L
H-HC-0.079700        0    -6.53472  -2.8497   -9.65461  L
H-HC-0.079700        0    -7.39129  -3.91449  -10.77767  L
H-H-0.419600         0    -6.82781  -0.7113   -12.5552  L
H-H-0.419600         0    -7.76047  -1.18819  -11.13902  L
N-N--0.415700        0    -3.38141  -2.95127  -10.74296  L
C-CT--0.051800       -1   -2.26337  -2.09922  -10.32827  L
C-C-0.597300         0    -2.84214  -0.68473  -10.05524  L
O-O--0.567900        0    -3.15487   0.03627  -11.00168  L
C-CT--0.110200       0    -1.1916   -2.09962  -11.43705  L
C-CT-0.353100        0    -0.02514  -1.11716  -11.206   L
C-CT--0.412100       0     0.78538  -1.46853  -9.95917  L
C-CT--0.412100       0     0.93135  -1.16315  -12.39993  L
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H-H-0.271900          0    -3.89522  -2.6552   -11.56983  L
H-H1-0.092200         0    -1.82177  -2.47658  -9.40578  L
H-HC-0.045700         0    -1.67529  -1.83311  -12.37864  L
H-HC-0.045700         0    -0.79495  -3.11041  -11.53838  L
H-HC--0.036100        0    -0.40262  -0.10116  -11.11066  L
H-HC-0.100000         0     1.15381  -2.4907   -10.03165  L
H-HC-0.100000         0     0.15602  -1.36163  -9.07699  L
H-HC-0.100000         0     1.62025  -0.77609  -9.85975  L
H-HC-0.100000         0     1.3389   -2.16703  -12.51663  L
H-HC-0.100000         0     1.74167  -0.45301  -12.24193  L
H-HC-0.100000         0     0.38883  -0.88393  -13.30315  L
N-N--0.347900         0    -3.01664  -0.29273  -8.77927  L
C-CT--0.263700        -1   -3.40227   1.08735  -8.37477  L
C-C-0.734100          0    -2.18408   2.00164  -8.53529  L
O-O--0.589400         0    -1.08285   1.53929  -8.82745  L
C-CT--0.000700        0    -3.99911   1.05174  -6.96196  L
C-CT-0.039000         0    -4.81089   2.30902  -6.61692  L
C-CT-0.048600         0    -5.62589   2.12325  -5.3412   L
N-N2--0.529500        0    -4.77985   2.00226  -4.14855  L
C-CA-0.807600         0    -5.23867   1.84872  -2.92593  L
N-N2--0.862700        0    -6.4763    1.58432  -2.67091  L
N-N2--0.862700        0    -4.47105   1.97074  -1.89428  L
H-H-0.274700          0    -2.62194  -0.9016   -8.07325  L
H-H1-0.156000         0    -4.16212   1.43976  -9.07547  L
H-HC-0.032700         0    -3.21049   0.89731  -6.22554  L
H-HC-0.032700         0    -4.68322   0.20652  -6.92855  L
H-HC-0.028500         0    -5.5029    2.52408  -7.43238  L
H-HC-0.028500         0    -4.15534   3.16642  -6.47789  L
H-H1-0.068700         0    -6.28168   1.25563  -5.44314  L
H-H1-0.068700         0    -6.23495   3.01483  -5.21622  L
H-H-0.345600          0    -3.80389   2.29293  -4.23996  L
H-H-0.447800          0    -6.77601   1.48761  -1.71057  L
H-H-0.447800          0    -7.03042   1.07244  -3.35715  L
H-H-0.447800          0    -4.87407   1.82834  -0.98095  L
H-H-0.447800          0    -3.52197   2.30715  -2.04869  L
N-N--0.415700         0    -2.36611   3.2939   -8.31533  L
C-CT--0.002400        -1   -1.28652   4.23912  -8.07693  L
C-C-0.597300          0    -1.71454   5.18568  -6.94994  L
O-O--0.567900         0    -2.84691   5.66446  -6.94539  L
C-CT--0.034300        0    -0.94647   5.00233  -9.36775  L
C-CA-0.011800         0    -0.40385   4.1271   -10.48725  L
C-CA--0.125600        0     0.9709    3.82787  -10.55681  L
C-CA--0.125600        0    -1.28052   3.57414  -11.4402  L
C-CA--0.170400        0     1.46665   2.99178  -11.57427  L
C-CA--0.170400        0    -0.7892    2.72765  -12.44949  L
C-CA--0.107200        0     0.585     2.44153  -12.5213  L
H-H-0.271900          0    -3.29219   3.62035  -8.08631  L
H-H1-0.097800         0    -0.40069   3.70227  -7.74657  L
H-HC-0.029500         0    -0.20582   5.76801  -9.13465  L
H-HC-0.029500         0    -1.84003   5.52088  -9.71985  L
H-HA-0.133000         0     1.64431   4.23348  -9.8206   L
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 H-HA-0.133000        0    -2.34035   3.77728  -11.38131  L
 H-HA-0.143000        0     2.51997   2.76571  -11.62189  L
 H-HA-0.143000        0    -1.47854   2.28583  -13.15546  L
 H-HA-0.129700        0     0.95353   1.78829  -13.29783  L
 N-N--0.516300        0    -0.83627   5.40535  -5.96804  L
 C-CT-0.038100        0    -1.19526   6.05521  -4.7049   L    H-HC
515   0.        0.
 C-C-0.536600         0    -0.38981   7.34547  -4.43239  L
 O-O--0.581900        0     0.1556    7.53608  -3.33533  L
 C-CT--0.030300       0    -1.04114   5.04816  -3.55789  H
 C-C-0.799400         0    -1.88849   3.78503  -3.58729  H
 O-O2--0.801400       0    -2.21453   3.34361  -2.35646  H
 O-O2--0.801400       0    -2.24402   3.12285  -4.52866  H
 H-H-0.293600         0     0.00546   4.85288  -5.97706  L
 H-H1-0.088000        0    -2.24456   6.35328  -4.73275  L
 H-HC--0.012200       0    -1.29419   5.57319  -2.6348   H
 H-HC--0.012200       0     0.00031   4.70651  -3.5127   H
 N-N--0.516300        0    -0.34779   8.25766  -5.40748  L
 C-CT-0.038100        0     0.26606   9.59051  -5.31663  L
 C-C-0.536600         0    -0.71748   10.68026  -4.86226  L
 O-O--0.581900        0    -0.79309   11.78213  -5.40242  L
 C-CT--0.030300       0     1.02686   9.96857  -6.60342  L
 C-C-0.799400         0     0.23468   9.89939  -7.91523  L
 O-O2--0.801400       0    -0.60275   8.97616  -8.05143  L
 O-O2--0.801400       0     0.58052   10.68911  -8.82125  L
 H-H-0.293600         0    -0.78767   8.07054  -6.311    L
 H-H1-0.088000        0     1.01309   9.53742  -4.53176  L
 H-HC--0.012200       0     1.88123   9.30649  -6.68939  L
 H-HC--0.012200       0     1.43623   10.97375  -6.48527  L
 N-N--0.415700        0    -1.38545   10.41869  -3.73834  L
 C-CT--0.038900       -1   -2.18213   11.39087  -2.96484  L
 C-C-0.597300         0    -1.30383   12.58676  -2.46058  L
 O-O--0.567900        0    -1.85969   13.5909  -2.02218  L
 C-CT-0.365400        0    -2.87669   10.69133  -1.80378  L
 O-OH--0.676100       0    -2.01134   9.81196  -1.10608  L
 C-CT--0.243800       -1   -3.98643   9.86384  -2.43546  L
 H-H-0.271900         0    -1.25001   9.50516  -3.32515  L
 H-H1-0.100700        0    -2.9387    11.82895  -3.61553  L
 H-H1-0.004300        0    -3.30038   11.41886  -1.11278  L
 H-HC-0.064200        0    -4.68186   10.51761  -2.96028  L
 H-HC-0.064200        0    -4.50971   9.35237  -1.63404  L
 H-HC-0.064200        0    -3.58623   9.11841  -3.12252  L
 H-HO-0.410200        0    -1.80035   10.24457  -0.24242  L
 N-N--0.415700        0     0.04907   12.55656  -2.57503  L
 C-CT-0.014300        -1    0.97571   13.7173  -2.44169  L
 C-C-0.597300         0     1.95332   13.82032  -3.63931  L
 O-O--0.567900        0     3.10515   13.38878  -3.50122  L
 C-CT--0.204100       0     1.61123   13.75813  -1.03957  L
 C-C-0.713000         0     2.51527   14.96922  -0.83949  L
 O-O--0.593100        0     2.74679   15.7909  -1.71301  L
 N-N--0.919100        0     3.08823   15.11986   0.32785  L
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H-H-0.271900         0     0.40061   11.72684  -3.03045  L
H-H1-0.104800        0     0.35966   14.61428  -2.47047  L
H-HC-0.079700        0     2.17178   12.85083  -0.85574  L
H-HC-0.079700        0     0.80877   13.80802  -0.30159  L
H-H-0.419600         0     3.6296    15.96054   0.41019  L
H-H-0.419600         0     2.85669   14.53682   1.12209  L
N-N--0.254800        0     1.53992   14.45005  -4.76909  L
C-CT--0.026600       -1    2.2812    14.47942  -6.04212  L
C-C-0.589600         0     3.65438   15.13249  -5.97033  L
O-O--0.574800        0     4.5108    14.88907  -6.81633  L
C-CT--0.007000       0     1.35439   15.1154  -7.08179  L
C-CT-0.018900        0     0.36445   15.91497  -6.24292  L
C-CT-0.019200        0     0.2429    15.0914  -4.96359  L
H-H1-0.064100        0     2.44467   13.44606  -6.34859  L
H-HC-0.025300        0     0.8206    14.32613  -7.61514  L
H-HC-0.025300        0     1.89212   15.74964  -7.78789  L
H-HC-0.021300        0    -0.59724   16.02354  -6.74544  L
H-HC-0.021300        0     0.78957   16.89197  -6.00849  L
H-H1-0.039100        0    -0.01586   15.75316  -4.13738  L
H-H1-0.039100        0    -0.52636   14.32799  -5.08886  L
N-N--0.415700        0     3.92427   15.93595  -4.94434  L
C-CT--0.025200       -1    5.13125   16.74761  -4.88981  L
C-C-0.597300         0     6.41883   16.05666  -4.44473  L
O-O--0.567900        0     7.30479   16.67783  -3.86285  L
H-H-0.271900         0     3.23356   16.02068  -4.20952  L
H-H1-0.069800        0     4.95357   17.57254  -4.20005  L
H-H1-0.069800        0     5.31439   17.1827  -5.87305  L
N-N--0.347900        0     6.5293    14.77472  -4.76821  L
C-CT--0.240000       -1    7.71323   13.91159  -4.69046  L
C-C-0.734100         0     7.61568   12.80478  -5.77704  L
O-O--0.589400        0     8.33828   11.80973  -5.6904   L
C-CT--0.009400       0     7.83654   13.35404  -3.25551  L
C-CT-0.018700        0     6.63965   12.45108  -2.96     L
C-CT--0.047900       0     6.57597   11.80617  -1.5845   L
C-CT--0.014300       0     5.47057   10.74877  -1.68306  L
N-N3--0.385400       0     4.11587   11.33732  -1.76854  L
H-H-0.274700         0     5.70449   14.42232  -5.24188  L
H-H1-0.142600        0     8.60096   14.50522  -4.91142  L
H-HC-0.036200        0     7.86188   14.17771  -2.53991  L
H-HC-0.036200        0     8.75987   12.78089  -3.16253  L
H-HC-0.010300        0     6.67998   11.63521  -3.6693   L
H-HC-0.010300        0     5.72117   13.01573  -3.11007  L
H-HC-0.062100        0     6.35194   12.54647  -0.81437  L
H-HC-0.062100        0     7.52466   11.31624  -1.36199  L
H-HP-0.113500        0     5.52844   10.11182  -0.80094  L
H-HP-0.113500        0     5.64587   10.13069  -2.56801  L
H-H-0.340000         0     3.50301   10.74592  -2.34191  L
H-H-0.340000         0     4.09771   12.19247  -2.32252  L
H-H-0.340000         0     3.72706   11.49224  -0.84995  L
N-N--0.516300        0     6.68542   12.91942  -6.7406   L
C-CT-0.039700        -1    6.14877   11.8198  -7.57159  L
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C-C-0.536600         0     6.29087   12.1312  -9.09119  L
O-O--0.581900        0     6.12056   13.27345  -9.50851  L
C-CT-0.056000        0     4.75176   11.3643  -7.07332  L
C-CT-0.013600        0     4.85647   11.06639  -5.55956  L
C-C-0.805400         0     3.90471   10.07517  -4.86756  L
O-O2--0.818800       0     3.05967   10.52219  -4.06228  L
O-O2--0.818800       0     4.24624   8.87293  -4.83424  L
H-H-0.293600         0     6.17702   13.79065  -6.85314  L
H-H1-0.110500        0     6.79835   10.95866  -7.41629  L
H-HC--0.017300       0     4.47837   10.47031  -7.61861  L
H-HC--0.017300       0     4.00744   12.13664  -7.25721  L
H-HC--0.042500       0     4.80729   12.02041  -5.03512  L
H-HC--0.042500       0     5.85092   10.65806  -5.4002   L
N-N--0.415700        0     6.7391    11.15122  -9.90665  L
C-CT--0.149000      -1     7.18637   11.32376  -11.30966  L
H-H-0.271900         0     6.82151   10.23151  -9.50207  L
H-H1-0.097600        0     7.97895   12.07257  -11.35246  L
H-H1-0.097600        0     6.34626   11.67265  -11.91397  L
H-H1-0.097600        0     7.55128   10.37758  -11.71018  L
C-CT--0.366200       0     10.3066   1.32599  -12.22104  L
C-C-0.597200         0     9.14544   0.88673  -11.36253  L
O-O--0.567900        0     9.3381    0.60059  -10.18558  L
H-HC-0.112300        0     10.87771   2.06779  -11.6666  L
H-HC-0.112300        0     9.95965   1.7585   -13.15685  L
H-HC-0.112300        0     10.93592   0.46029  -12.41895  L
N-N--0.415700        0     7.94646   0.85384  -11.95111  L
C-CT--0.059700      -1     6.70314   0.39315  -11.30954  L
C-C-0.597300         0     5.90814  -0.50602  -12.27511  L
O-O--0.567900        0     6.04343  -1.72335  -12.2084  L
C-CT-0.130300        0     5.87952   1.56506  -10.7028  L
C-CT--0.043000       0     6.71309   2.36096  -9.66565  L
C-CT--0.320400       0     4.59705   1.03195  -10.03092  L
C-CT--0.066000       0     6.01319   3.58622  -9.06882  L
H-H-0.271900         0     7.9222    1.08576  -12.93019  L
H-H1-0.086900        0     6.98572  -0.2538   -10.47966  L
H-HC-0.018700        0     5.59257   2.2453   -11.50649  L
H-HC-0.023600        0     7.61482   2.7378   -10.14549  L
H-HC-0.023600        0     7.01396   1.69671  -8.8537   L
H-HC-0.088200        0     3.9959    0.4428   -10.72257  L
H-HC-0.088200        0     3.97297   1.86006  -9.69848  L
H-HC-0.088200        0     4.85298   0.4103   -9.1731   L
H-HC-0.018600        0     5.17655   3.28669  -8.44069  L
H-HC-0.018600        0     5.6572    4.23611  -9.86889  L
H-HC-0.018600        0     6.7241    4.1388   -8.4535   L
N-N--0.415700        0     5.10278   0.07082  -13.18023  L
C-CT--0.149000      -1     4.25868  -0.667    -14.12473  L
H-H-0.271900         0     5.03264   1.07564  -13.16043  L
H-H1-0.097600        0     3.73781  -1.47339  -13.60314  L
H-H1-0.097600        0     4.87646  -1.10558  -14.91012  L
H-H1-0.097600        0     3.51946  -0.00143  -14.57329  L
C-CT--0.366200      -1    -5.01133   16.98003  -3.212    L
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C-C-0.597200         0    -5.56898   16.20199  -2.03301  L
O-O--0.567900        0    -5.3617    16.61802  -0.89658  L
H-HC-0.112300        0    -5.82843   17.39508  -3.79708  L
H-HC-0.112300        0    -4.39918   16.31608  -3.82061  L
H-HC-0.112300        0    -4.38786   17.78754  -2.8322   L
N-N--0.254800        0    -6.32844   15.12158  -2.27757  L
C-CT--0.026600       -1   -7.00768   14.37161  -1.22685  L
C-C-0.589600         0    -6.1444    13.27683  -0.60493  L
O-O--0.574800        0    -5.59937   12.40562  -1.28038  L
C-CT--0.007000       0    -8.22032   13.75983  -1.93835  L
C-CT-0.018900        0    -7.70518   13.48719  -3.35373  L
C-CT-0.019200        0    -6.73178   14.64205  -3.59509  L
H-H1-0.064100        0    -7.3582    15.04912  -0.44747  L
H-HC-0.025300        0    -9.02398   14.49643  -1.98176  L
H-HC-0.025300        0    -8.57226   12.85024  -1.45184  L
H-HC-0.021300        0    -8.51561   13.48431  -4.08302  L
H-HC-0.021300        0    -7.16732   12.53918  -3.38431  L
H-H1-0.039100        0    -5.86921   14.29274  -4.1646   L
H-H1-0.039100        0    -7.24312   15.43963  -4.13509  L
N-N--0.415700        0    -6.09112   13.31277   0.71918  L
C-CT--0.023700       -1   -5.2437    12.47718   1.5572   L
C-C-0.597300         0    -5.43019   10.95167   1.41663  L
O-O--0.567900        0    -6.50905   10.47193   1.05896  L
C-CT-0.034200        0    -5.50446   12.84646   3.03127  L
C-CT-0.001800        0    -5.0523    14.26204   3.41896  L
S-S--0.273700        0    -3.26257   14.50136   3.60376  L
C-CT--0.053600       -1   -2.96044   13.57137   5.13418  L
H-H-0.271900         0    -6.5812    14.07012   1.16283  L
H-H1-0.088000        0    -4.20054   12.69954   1.32116  L
H-HC-0.024100        0    -4.99932   12.13283   3.68231  L
H-HC-0.024100        0    -6.5747    12.75886   3.22582  L
H-H1-0.044000        0    -5.51963   14.51798   4.37006  L
H-H1-0.044000        0    -5.41758   14.97041   2.67544  L
H-H1-0.068400        0    -3.18347   12.51553   4.97855  L
H-H1-0.068400        0    -3.58415   13.96186   5.93759  L
H-H1-0.068400        0    -1.91037   13.66291   5.41136  L
N-N--0.415700        0    -4.38271   10.19758   1.78241  L
C-CT--0.001400       -1   -4.25937   8.74375    1.63352  L
C-C-0.597300         0    -5.5099    7.88488    1.93554  L
O-O--0.567900        0    -6.09698   7.3818     0.98336  L
C-CT--0.015200       0    -2.99092   8.20191    2.313    L
C-CA--0.001100       0    -2.94416   6.69876    2.53606  L
C-CA--0.190600       0    -3.29204   5.79362    1.51321  L
C-CA--0.190600       0    -2.65087   6.21237    3.81972  L
C-CA--0.234100       0    -3.36629   4.41366    1.79353  L
C-CA--0.234100       0    -2.773     4.84424    4.11039  L
C-C-0.322600         0    -3.13406   3.93834    3.09942  L
O-OH--0.557900       0    -3.27958   2.61714    3.37373  L
H-H-0.271900         0    -3.52259   10.68252    2.01732  L
H-H1-0.087600        0    -4.09107   8.58897    0.5679   L
H-HC-0.029500        0    -2.88289   8.70139    3.27555  L
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H-HC-0.029500        0    -2.13549   8.45564   1.69351  L
H-HA-0.169900        0    -3.58061   6.16949   0.53909  L
H-HA-0.169900        0    -2.41722   6.90386   4.6155   L
H-HA-0.165600        0    -3.68408   3.70462   1.0465   L
H-HA-0.165600        0    -2.66699   4.50483   5.12762  L
H-HO-0.399200        0    -3.59133   2.49892   4.29308  L
N-N--0.516300        0    -5.86903   7.59594   3.19342  L
C-CT-0.038100        -1   -6.81724   6.5184    3.57428  L
C-C-0.536600         0    -8.21984   6.72616   3.00156  L
O-O--0.581900        0    -8.86875   5.76075   2.60882  L
C-CT--0.030300       0    -6.8829    6.37753   5.10689  L
C-C-0.799400         0    -5.60305   5.78069   5.70509  L
O-O2--0.801400       0    -5.46739   4.53326   5.66622  L
O-O2--0.801400       0    -4.75342   6.56921   6.18971  L
H-H-0.293600         0    -5.36881   8.07747   3.93637  L
H-H1-0.088000        0    -6.4396    5.57447   3.18713  L
H-HC--0.012200       0    -7.71346   5.71813   5.36189  L
H-HC--0.012200       0    -7.09007   7.3502    5.55616  L
N-N--0.415700        0    -8.67019   7.98035   2.91416  L
C-CT--0.002400       0    -9.85943   8.37143   2.15595  L
C-C-0.597300         0    -9.75504   7.92362   0.68971  L
O-O--0.567900        0    -10.60466   7.18191   0.1973   L
C-CT--0.034300       0    -10.06144   9.89022   2.27016  L
C-CA-0.011800        0    -11.11704   10.43211   1.32409  L
C-CA--0.125600       0    -12.48365   10.25535   1.61072  L
C-CA--0.125600       0    -10.73068   11.0554   0.12156  L
C-CA--0.170400       0    -13.45866   10.70423   0.70139  L
C-CA--0.170400       0    -11.70488   11.50194  -0.78823  L
C-CA--0.107200       0    -13.06948   11.32698  -0.49806  L
H-H-0.271900         0    -8.03211   8.69488   3.23352  L
H-H1-0.097800        0    -10.73012   7.87193   2.5825   L
H-HC-0.029500        0    -9.11585   10.39398   2.06242  L
H-HC-0.029500        0    -10.34387   10.13287   3.29536  L
H-HA-0.133000        0    -12.78541   9.75593   2.52036  L
H-HA-0.133000        0    -9.6819    11.16518  -0.12001  L
H-HA-0.143000        0    -14.50669   10.55438   0.91768  L
H-HA-0.143000        0    -11.39972   11.96094  -1.71787  L
H-HA-0.129700        0    -13.81821   11.65816  -1.20348  L
N-N--0.415700        0    -8.71712   8.36617  -0.01789  L
C-CT--0.038900       -1   -8.52903   8.06655  -1.44156  L
C-C-0.597300         0    -8.35861   6.58642  -1.73659  L
O-O--0.567900        0    -8.99385   6.04118  -2.63548  L
C-CT-0.365400        0    -7.37624   8.89474  -2.01965  L
O-OH--0.676100       0    -7.62697   10.26508  -1.78964  L
C-CT--0.243800       0    -7.23328   8.72577  -3.53298  L
H-H-0.271900         0    -8.04099   8.97667   0.42994  L
H-H1-0.100700        0    -9.43358   8.38079  -1.96217  L
H-H1-0.004300        0    -6.45514   8.60154  -1.52237  L
H-HC-0.064200        0    -8.18446   8.94122  -4.02022  L
H-HC-0.064200        0    -6.92681   7.70783  -3.77296  L
H-HC-0.064200        0    -6.4813    9.41317  -3.91638  L
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H-HO-0.410200        0    -6.79152   10.69359  -1.54699  L
N-N--0.415700        0    -7.52436   5.93485  -0.93856  L
C-CT--0.058100       -1   -7.38971   4.49253  -0.80284  L
C-C-0.597300         0    -8.73927   3.80157  -0.66858  L
O-O--0.567900        0    -9.05458   2.94632  -1.49522  L
C-CT--0.007400       0    -6.45915   4.26614   0.38838  L
C-CC-0.186800        0    -6.40224   2.87256   0.93462  L
N-NB--0.543200       0    -6.49938   1.70966   0.18348  L
C-CW--0.220700       0    -6.29247   2.54904   2.25142  L
C-CR-0.163500        0    -6.49458   0.69706   1.05462  L
N-NA--0.279500       0    -6.34946   1.17705   2.29922  L
H-H-0.271900         0    -7.0747    6.50961  -0.23286  L
H-H1-0.136000        0    -6.92163   4.08874  -1.70037  L
H-HC-0.036700        0    -6.78207   4.90702   1.20119  L
H-HC-0.036700        0    -5.46294   4.57465   0.08503  L
H-H4-0.186200        0    -6.21262   3.23129   3.08953  L
H-H-0.333900         0    -6.33911   0.59031   3.13185  L
H-H5-0.143500        0    -6.61172  -0.34633   0.78682  L
N-N--0.415700        0    -9.53946   4.18218   0.33285  L
C-CT-0.021300        -1   -10.83997   3.565     0.54448  L
C-C-0.597300         0    -11.75113   3.61075  -0.66035  L
O-O--0.567900        0    -12.36045   2.60833  -1.02966  L
C-CT--0.123100       0    -11.496    3.96868   1.88303  L
S-SH--0.311900       0    -12.58364   5.42033   1.79802  L
H-H-0.271900         0    -9.23026   4.89822   0.98193  L
H-H1-0.112400        0    -10.62487   2.50103   0.65442  L
H-H1-0.111200        0    -10.72524   4.13804   2.63399  L
H-H1-0.111200        0    -12.0993   3.12739   2.22826  L
H-HS-0.193300        0    -11.67655   6.2565    1.27582  L
N-N--0.415700        0    -11.79211   4.77311  -1.29003  L
C-CT--0.059700       -1   -12.6058   4.99546  -2.45735  L
C-C-0.597300         0    -12.11344   4.28143  -3.71728  L
O-O--0.567900        0    -12.9261   3.66039  -4.40039  L
C-CT-0.130300        0    -12.82894   6.52116  -2.64059  L
C-CT--0.043000       0    -14.16257   6.97329  -1.99511  L
C-CT--0.320400       -1   -12.73369   7.02236  -4.08734  L
C-CT--0.066000       -1   -15.45327   6.57376  -2.74084  L
H-H-0.271900         0    -11.25465   5.53721  -0.89466  L
H-H1-0.086900        0    -13.57783   4.5478   -2.25246  L
H-HC-0.018700        0    -12.03364   7.04309  -2.10469  L
H-HC-0.023600        0    -14.14934   8.0607   -1.90863  L
H-HC-0.023600        0    -14.20976   6.57212  -0.98147  L
H-HC-0.088200        0    -11.71454   6.90741  -4.45774  L
H-HC-0.088200        0    -12.98309   8.08284  -4.12539  L
H-HC-0.088200        0    -13.41774   6.47176  -4.73482  L
H-HC-0.018600        0    -16.31704   6.88671  -2.15402  L
H-HC-0.018600        0    -15.49558   5.4935   -2.87916  L
H-HC-0.018600        0    -15.49761   7.06523  -3.71254  L
N-N--0.415700        0    -10.82034   4.36473  -4.04644  L
C-CT--0.024900       -1   -10.25015   3.63027  -5.18147  L
C-C-0.597300         0    -10.51968   2.1208   -5.0062   L
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O-O--0.567900        0    -10.92882   1.48373  -5.96877  L
C-CT-0.211700        0    -8.75949    3.89449  -5.32588  L
O-OH--0.654600       0    -8.30606    3.33938  -6.54733  L
H-H-0.271900         0    -10.20877    4.90214  -3.44003  L
H-H1-0.084300        0    -10.75023    3.95902  -6.09319  L
H-H1-0.035200        0    -8.23112    3.44656  -4.48315  L
H-H1-0.035200        0    -8.57439    4.96966  -5.33134  L
H-HO-0.427500        0    -8.85909    2.58057  -6.78344  L
N-N--0.516300        0    -10.32126    1.54747  -3.80725  L
C-CT-0.038100        -1   -10.57736    0.12011  -3.52182  L
C-C-0.536600         0    -12.05781  -0.27766  -3.62924  L
O-O--0.581900        0    -12.3934   -1.23464  -4.33199  L
C-CT--0.030300       0    -9.96824   -0.30408  -2.17433  L
C-C-0.799400         0    -8.49792   -0.69703  -2.31999  L
O-O2--0.801400       0    -7.92125   -0.50745  -3.41478  L
O-O2--0.801400       0    -7.90001   -1.19254  -1.33812  L
H-H-0.293600         0    -9.97769    2.12593  -3.04722  L
H-H1-0.088000        0    -10.09296  -0.45351  -4.31053  L
H-HC--0.012200       0    -10.5088   -1.1695   -1.79062  L
H-HC--0.012200       0    -10.07441    0.49791  -1.44313  L
N-N--0.415700        0    -12.94505    0.45738  -2.95471  L
C-CT-0.033700        -1   -14.39936    0.33609  -3.07782  L
C-C-0.597300         0    -14.8682    0.34678  -4.5446   L
O-O--0.567900        0    -15.69295  -0.474    -4.94133  L
C-CT--0.182500       -1   -15.00604    1.50129  -2.35613  L
H-H-0.271900         0    -12.58768    1.22091  -2.38936  L
H-H1-0.082300        0    -14.72908  -0.59712  -2.62024  L
H-HC-0.060300        0    -14.74176    1.4582   -1.29904  L
H-HC-0.060300        0    -16.09279    1.45599  -2.43975  L
H-HC-0.060300        0    -14.65658    2.44465  -2.77492  L
N-N--0.415700        0    -14.37417    1.31678  -5.32084  L
C-CT--0.025200       -1   -14.74694    1.56315  -6.71023  L
C-C-0.597300         0    -14.26012    0.49856  -7.68973  L
O-O--0.567900        0    -14.99962    0.09989  -8.58401  L
H-H-0.271900         0    -13.7144    1.95837  -4.89294  L
H-H1-0.069800        0    -14.33501    2.52179  -7.02284  L
H-H1-0.069800        0    -15.83316    1.61461  -6.7833   L
N-N--0.516300        0    -13.01168    0.0665   -7.53003  L
C-CT-0.039700        -1   -12.38052  -1.02894  -8.27102  L
C-C-0.536600         0    -13.11651  -2.37032  -8.09288  L
O-O--0.581900        0    -13.25081  -3.13407  -9.04535  L
C-CT-0.056000        0    -10.91928  -1.0898   -7.79863  L
C-CT-0.013600        0    -10.04054  -2.18318  -8.41415  L
C-C-0.805400         0    -9.58673   -1.89172  -9.84589  L
O-O2--0.818800       0    -9.59315   -2.82882  -10.67486  L
O-O2--0.818800       0    -9.07619   -0.77724  -10.09184  L
H-H-0.293600         0    -12.45085    0.50453  -6.80607  L
H-H1-0.110500        0    -12.39015  -0.79644  -9.33684  L
H-HC--0.017300       0    -10.93558  -1.24134  -6.72237  L
H-HC--0.017300       0    -10.44763  -0.12367  -7.97897  L
H-HC--0.042500       0    -10.56998  -3.13062  -8.36211  L
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H-HC--0.042500       0    -9.14136  -2.27734  -7.80269  L
N-N--0.415700        0    -13.57854  -2.66663  -6.87297  L
C-CT--0.025200       -1   -14.28437  -3.90808  -6.5206   L
C-C-0.597300         0    -13.54101  -4.76753  -5.51381  L
O-O--0.567900        0    -13.88909  -5.9394   -5.35142  L
H-H-0.271900         0    -13.46062  -1.95024  -6.16604  L
H-H1-0.069800        0    -14.45799  -4.50988  -7.41316  L
H-H1-0.069800        0    -15.25262  -3.64967  -6.0937   L
N-N--0.415700        0    -12.5287  -4.21027  -4.83203  L
C-CT--0.059700       -1   -11.8012  -4.9171   -3.77697  L
C-C-0.597300         0    -12.82627  -5.45437  -2.77324  L
O-O--0.567900        0    -13.7511  -4.74811  -2.37711  L
C-CT-0.130300        0    -10.73805  -4.02356  -3.08454  L
C-CT--0.043000       0    -9.41188  -3.96213  -3.86147  L
C-CT--0.320400       0    -10.32388  -4.52397  -1.68305  L
C-CT--0.066000       0    -9.4858   -3.39995  -5.27398  L
H-H-0.271900         0    -12.36925  -3.21722  -4.96332  L
H-H1-0.086900        0    -11.30011  -5.76112  -4.23241  L
H-HC-0.018700        0    -11.14148  -3.02041  -2.97112  L
H-HC-0.023600        0    -9.00365  -4.96264  -3.9185   L
H-HC-0.023600        0    -8.71286  -3.34553  -3.30009  L
H-HC-0.088200        0    -9.57337  -3.85573  -1.25664  L
H-HC-0.088200        0    -9.91373  -5.53287  -1.74463  L
H-HC-0.088200        0    -11.17498  -4.51716  -1.01077  L
H-HC-0.018600        0    -8.485    -3.36417  -5.70164  L
H-HC-0.018600        0    -9.8888   -2.39463  -5.23164  L
H-HC-0.018600        0    -10.11282  -4.02784  -5.90287  L
N-N--0.415700        0    -12.64929  -6.7061   -2.34851  L
C-CT--0.025200       -1   -13.5072  -7.34049  -1.33983  L
C-C-0.597300         0    -12.95497  -7.27273   0.06711  L
O-O--0.567900        0    -13.68142  -7.05875   1.03547  L
H-H-0.271900         0    -11.90888  -7.2195   -2.80951  L
H-H1-0.069800        0    -13.64419  -8.38874  -1.60071  L
H-H1-0.069800        0    -14.49162  -6.86984  -1.34137  L
N-N--0.415700        0    -11.6482  -7.47414   0.16262  L
C-CT--0.058100       -1   -10.89714  -7.4635    1.3996   L
C-C-0.597300         0    -9.51595  -6.82879   1.1307   L
O-O--0.567900        0    -8.78157  -7.31804   0.2734   L
C-CT--0.007400       0    -10.75706  -8.90571   1.91674  L
C-CC-0.186800        0    -12.05786  -9.48368   2.42642  L
N-NB--0.543200       0    -12.66183  -9.18728   3.65165  L
C-CW--0.220700       0    -12.8732  -10.32076   1.72238  L
C-CR-0.163500        0    -13.83295  -9.83897   3.65057  L
N-NA--0.279500       0    -13.98579  -10.53215   2.50819  L
H-H-0.271900         0    -11.12748  -7.60396  -0.693    L
H-H1-0.136000        0    -11.41562  -6.86983   2.15419  L
H-HC-0.036700        0    -10.02149  -8.93231   2.71821  L
H-HC-0.036700        0    -10.37571  -9.53994   1.11496  L
H-H4-0.186200        0    -12.6852  -10.69501   0.7263   L
H-H-0.333900         0    -14.80204  -11.07225   2.26195  L
H-H5-0.143500        0    -14.55583  -9.79933   4.45531  L
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N-N--0.415700        0    -9.16128  -5.72646   1.80331  L
C-CT--0.024900       -1   -7.899    -4.99678   1.56891  L
C-C-0.597300         0    -6.70843  -5.62565   2.29433  L
O-O--0.567900        0    -6.74702  -5.87898   3.49782  L
C-CT-0.211700        0    -8.02571  -3.50299   1.89526  L
O-OH--0.654600       0    -6.74869  -2.8761    1.86965  L
H-H-0.271900         0    -9.77497  -5.42894   2.55396  L
H-H1-0.084300        0    -7.68636  -5.04744   0.50035  L
H-H1-0.035200        0    -8.47514  -3.38594   2.8746   L
H-H1-0.035200        0    -8.67782  -3.0265    1.16095  L
H-HO-0.427500        0    -6.76726  -2.11474   2.4792   L
N-N--0.415700        0    -5.62028  -5.84261   1.5531   L
C-CT--0.051800       -1   -4.31948  -6.23951   2.08802  L
C-C-0.597300         0    -3.44092  -5.02188   2.31547  L
O-O--0.567900        0    -3.23339  -4.23433   1.39316  L
C-CT--0.110200       0    -3.62976  -7.22306   1.11815  L
C-CT-0.353100        0    -4.1462   -8.67511   1.1329   L
C-CT--0.412100       0    -5.52197  -8.8457    0.48758  L
C-CT--0.412100       0    -3.16408  -9.55904   0.35722  L
H-H-0.271900         0    -5.70039  -5.65209   0.56601  L
H-H1-0.092200        0    -4.45782  -6.7432    3.04797  L
H-HC-0.045700        0    -2.57785  -7.25883   1.3919   L
H-HC-0.045700        0    -3.68236  -6.83411   0.10407  L
H-HC--0.036100       0    -4.18718  -9.03084   2.16266  L
H-HC-0.100000        0    -5.52226  -8.43395  -0.52228  L
H-HC-0.100000        0    -6.28305  -8.3436    1.08237  L
H-HC-0.100000        0    -5.78429  -9.90165   0.44399  L
H-HC-0.100000        0    -2.17459  -9.49985   0.80984  L
H-HC-0.100000        0    -3.10921  -9.23068  -0.68127  L
H-HC-0.100000        0    -3.50093  -10.59518   0.38536  L
N-N--0.415700        0    -2.88483  -4.90607   3.51408  L
C-CT-0.021300        -1   -1.94087  -3.84982   3.84775  L
C-C-0.597300         0    -0.80545  -4.3654    4.74965  L
O-O--0.567900        0    -0.81771  -5.52297   5.17075  L
C-CT--0.123100       0    -2.74409  -2.70958   4.48303  L
S-SH--0.311900       0    -1.81062  -1.15819   4.44736  L
H-H-0.271900         0    -3.1339   -5.57109   4.23875  L
H-H1-0.112400        0    -1.47699  -3.47057   2.93386  L
H-H1-0.111200        0    -3.01185  -2.96489   5.51009  L
H-H1-0.111200        0    -3.65912  -2.56004   3.90926  L
H-HS-0.193300        0    -2.69487  -0.44654   5.16094  L
N-N--0.415700        0     0.18671  -3.53332   5.06905  L
C-CT--0.038900       -1    1.28932  -3.90849   5.96773  L
C-C-0.597300         0     1.42221  -3.00482   7.16971  L
O-O--0.567900        0     0.77294  -1.97329   7.31443  L
C-CT-0.365400        0     2.64809  -4.07121   5.2571   L
O-OH--0.676100       0     3.10808  -2.87695   4.66219  L
C-CT--0.243800       0     2.61658  -5.18641   4.21561  L
H-H-0.271900         0     0.10977  -2.57725   4.74191  L
H-H1-0.100700        0     1.06154  -4.88789   6.38848  L
H-H1-0.004300        0     3.39315  -4.37042   5.99438  L
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H-HC-0.064200        0     1.92874  -4.94277   3.40771  L
H-HC-0.064200        0     2.28842  -6.11553   4.68303  L
H-HC-0.064200        0     3.61438  -5.32841   3.81062  L
H-HO-0.410200        0     3.45956  -2.29116   5.37217  L
N-N--0.415700        0     2.25331  -3.49171   8.08256  L
C-CT--0.051800       -1    2.16935  -3.18785   9.48842  L
C-C-0.597300         0     2.2559   -1.68745   9.86177  L
O-O--0.567900        0     1.68591  -1.28975   10.86814  L
C-CT--0.110200       0     3.17326  -4.05584   10.21589  L
C-CT-0.353100        0     2.87028  -4.12767   11.71417  L
C-CT--0.412100       0     1.52746  -4.77207   12.07    L
C-CT--0.412100       -1    3.9611   -5.02282   12.24061  L
H-H-0.271900         0     2.69814  -4.3595    7.84143  L
H-H1-0.092200        0     1.16726  -3.49454   9.78936  L
H-HC-0.045700        0     4.17075  -3.64372   10.05485  L
H-HC-0.045700        0     3.13392  -5.0659    9.80282  L
H-HC--0.036100       0     2.95938  -3.1492    12.18293  L
H-HC-0.100000        0     1.40722  -5.72877   11.56306  L
H-HC-0.100000        0     0.70831  -4.11078   11.79474  L
H-HC-0.100000        0     1.4634   -4.92145   13.14887  L
H-HC-0.100000        0     3.85187  -5.11006   13.32249  L
H-HC-0.100000        0     4.93979  -4.58879   12.03842  L
H-HC-0.100000        0     3.89199  -6.01924   11.80423  L
N-N--0.516300        0     2.93557  -0.8481    9.07587  L
C-CT-0.039700        -1    3.06623   0.60703   9.31155  L
C-C-0.536600         0     1.82059   1.45766   8.97424  L
O-O--0.581900        0     1.90291   2.68801   8.9473   L
C-CT-0.056000        0     4.32224   1.11044   8.56278  L
C-CT-0.013600        0     4.31458   0.95961   7.02696  L
C-C-0.805400         0     4.94056  -0.34976   6.53121  L
O-O2--0.818800       0     4.29454  -1.42424   6.57894  L
O-O2--0.818800       0     6.13002  -0.3397    6.1199   L
H-H-0.293600         0     3.28299  -1.22298   8.19771  L
H-H1-0.110500        0     3.23567   0.76552   10.37768  L
H-HC--0.017300       0     5.19997   0.59744   8.95986  L
H-HC--0.017300       0     4.45312   2.16779   8.79601  L
H-HC--0.042500       0     4.91295   1.77374   6.61672  L
H-HC--0.042500       0     3.30089   1.06383   6.64206  L
N-N--0.415700        0     0.67379   0.81181   8.75176  L
C-CT--0.002400       -1   -0.63945   1.43305   8.54144  L
C-C-0.597300         0    -1.77674   0.8011    9.35868  L
O-O--0.567900        0    -2.95213   1.12454   9.17354  L
C-CT--0.034300       0    -1.01775   1.26491   7.06305  L
C-CA-0.011800        0    -0.08832   1.8446    6.0206   L
C-CA--0.125600       0    -0.22282   3.19118   5.64656  L
C-CA--0.125600       0     0.80754   1.01155   5.32714  L
C-CA--0.170400       0     0.47735   3.68633   4.53559  L
C-CA--0.170400       0     1.54838   1.51946   4.24809  L
C-CA--0.107200       0     1.36732   2.85194   3.83808  L
H-H-0.271900         0     0.73064  -0.1959    8.68276  L
H-H1-0.097800        0    -0.59443   2.49479   8.78293  L
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H-HC-0.029500        0    -1.99444   1.71943   6.90159  L
H-HC-0.029500        0    -1.13344   0.19835   6.86905  L
H-HA-0.133000        0    -0.89893   3.83324   6.19113  L
H-HA-0.133000        0     0.90256  -0.02775   5.60451  L
H-HA-0.143000        0     0.31512   4.708     4.22639  L
H-HA-0.143000        0     2.22303   0.86826   3.71345  L
H-HA-0.129700        0     1.9095    3.23064   2.98396  L
N-N--0.415700        0    -1.41885  -0.11472   10.24788  L
C-CT--0.003100      -1    -2.28646  -0.98329   11.0257  L
C-C-0.597300         0    -3.53016  -0.27806   11.62731  L
O-O--0.567900        0    -4.67057  -0.60833   11.31827  L
C-CT--0.003600       0    -1.37055  -1.56932   12.12048  L
C-CT--0.064500       0    -2.03145  -2.30563   13.29846  L
C-C-0.695100         0    -1.10133  -2.34177   14.50995  L
O-O--0.608600        0    -0.64474  -3.3874    14.94293  L
N-N--0.940700        0    -0.78179  -1.21536   15.11605  L
H-H-0.271900         0    -0.42226  -0.20294   10.40356  L
H-H1-0.085000        0    -2.66101  -1.78688   10.40608  L
H-HC-0.017100        0    -0.7879   -0.74304   12.53137  L
H-HC-0.017100        0    -0.66433  -2.251     11.6488  L
H-HC-0.035200        0    -2.27901  -3.32271   12.99342  L
H-HC-0.035200        0    -2.94931  -1.81428   13.61314  L
H-H-0.425100         0    -0.15015  -1.33118   15.88226  L
H-H-0.425100         0    -1.04828  -0.28447   14.78481  L
N-N--0.516300        0    -3.31395   0.6396    12.56343  L
C-CT-0.038100       -1    -4.28374   1.51803   13.25511  L
C-C-0.536600         0    -4.85449   2.58667   12.32012  L
O-O--0.581900        0    -6.04651   2.88782   12.3738  L
C-CT--0.030300       0    -3.55533   2.16228   14.45312  L
C-C-0.799400         0    -2.09169   2.46171   14.10925  L
O-O2--0.801400       0    -1.83694   3.46289   13.40389  L
O-O2--0.801400       0    -1.25529   1.54981   14.32829  L
H-H-0.293600         0    -2.33563   0.78454   12.79061  L
H-H1-0.088000        0    -5.12177   0.92678   13.62514  L
H-HC--0.012200       0    -3.58146   1.46299   15.29083  L
H-HC--0.012200       0    -4.0683    3.07554   14.75937  L
N-N--0.415700        0    -4.00594   3.13134   11.44369  L
C-CT-0.014300       -1    -4.35528   4.14431   10.45153  L
C-C-0.597300         0    -5.60123   3.80488   9.6342   L
O-O--0.567900        0    -6.3843    4.68953   9.28937  L
C-CT--0.204100       0    -3.14948   4.45775   9.54422  L
C-C-0.713000         0    -2.16352   5.46649   10.10676  L
O-O--0.593100        0    -1.75552   6.38754   9.41912  L
N-N--0.919100        0    -1.70081   5.34561   11.32964  L
H-H-0.271900         0    -3.04537   2.82939   11.52063  L
H-H1-0.104800        0    -4.61266   5.06027   10.98696  L
H-HC-0.079700        0    -3.52782   4.88212   8.61185  L
H-HC-0.079700        0    -2.61095   3.55424   9.28964  L
H-H-0.419600         0    -1.06643   6.07515   11.58746  L
H-H-0.419600         0    -1.95689   4.62003   12.003   L
N-N--0.347900        0    -5.80063   2.51552   9.35608  L
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C-CT--0.263700       -1   -6.94692   2.01478   8.60602  L
C-C-0.734100         0    -8.34209   2.33597   9.15916  L
O-O--0.589400        0    -9.3277    2.14005   8.45119  L
C-CT--0.000700       0    -6.77409   0.51066   8.32833  L
C-CT-0.039000        0    -7.36939  -0.3706    9.43071  L
C-CT-0.048600        0    -6.96578  -1.83407   9.26794  L
N-N2--0.529500       0    -7.63877  -2.63031   10.30014  L
C-CA-0.807600        0    -7.12965  -3.00278   11.44919  L
N-N2--0.862700       0    -5.8575   -3.09203   11.67653  L
N-N2--0.862700       0    -7.91726  -3.23863   12.44895  L
H-H-0.274700         0    -5.08222   1.87142   9.66988  L
H-H1-0.156000        0    -6.91426   2.51762   7.63751  L
H-HC-0.032700        0    -5.712     0.28453   8.21828  L
H-HC-0.032700        0    -7.27502   0.26791   7.38965  L
H-HC-0.028500        0    -8.4579   -0.30793   9.39761  L
H-HC-0.028500        0    -7.03084  -0.01326   10.4036  L
H-H1-0.068700        0    -5.88371  -1.90523   9.3547   L
H-H1-0.068700        0    -7.25717  -2.19656   8.28539  L
H-H-0.345600         0    -8.64765  -2.69414   10.24993  L
H-H-0.447800         0    -5.48695  -2.15218   11.76072  L
H-H-0.447800         0    -5.37699  -3.45823   10.84485  L
H-H-0.447800         0    -7.48975  -3.47357   13.31967  L
H-H-0.447800         0    -8.89166  -2.95794   12.34684  L
N-N--0.415700        0    -8.46081   2.79971   10.39976  L
C-CT--0.149000       -1   -9.74648   3.1467    10.97952  L
H-H-0.271900         0    -7.60884   2.92396   10.93611  L
H-H1-0.097600        0    -10.32299   3.75906   10.2851  L
H-H1-0.097600        0    -9.5926    3.70105   11.90599  L
H-H1-0.097600        0    -10.30211   2.23243   11.19816  L
C-CT--0.366200       -1   -9.94036   6.34993   8.7732   L
C-C-0.597200         0    -10.65684   5.60838   7.66881  L
O-O--0.567900        0    -11.83526   5.86244   7.458    L
H-HC-0.112300        0    -9.12391   5.74422   9.16707  L
H-HC-0.112300        0    -10.64788   6.57508   9.56827  L
H-HC-0.112300        0    -9.53957   7.27663   8.36687  L
N-N--0.415700        0    -9.96961   4.68507   6.99284  L
C-CT--0.001400       -1   -10.49644   3.83934   5.90139  L
C-C-0.597300         0    -11.83131   3.1439    6.20595  L
O-O--0.567900        0    -12.70479   3.005     5.34678  L
C-CT--0.015200       0    -9.36365   2.93732   5.35897  L
C-CA--0.001100       0    -9.76023   1.7024    4.571    L
C-CA--0.190600       0    -10.36343   0.61528   5.23205  L
C-CA--0.190600       0    -9.45967   1.60622   3.19787  L
C-CA--0.234100       0    -10.71289  -0.54016   4.51323  L
C-CA--0.234100       0    -9.76538   0.43169   2.48293  L
C-C-0.322600         0    -10.40157  -0.63815   3.14216  L
O-OH--0.557900       0    -10.72841  -1.76564   2.46745  L
H-H-0.271900         0    -9.00531   4.55143   7.25829  L
H-H1-0.087600        0    -10.74187   4.51776   5.08275  L
H-HC-0.029500        0    -8.73158   2.60065   6.17305  L
H-HC-0.029500        0    -8.72166   3.55831   4.7328   L
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H-HA-0.169900        0    -10.5668   0.67533   6.29209  L
H-HA-0.169900        0    -8.97642   2.42973   2.69085  L
H-HA-0.165600        0    -11.20496  -1.36023   5.00756  L
H-HA-0.165600        0    -9.5308    0.34112   1.43093  L
H-HO-0.399200        0    -11.63542  -1.99978   2.73384  L
N-N--0.516300        0    -12.00358   2.7315    7.45419  L
C-CT-0.038100        -1   -13.23396   2.17096   7.98988  L
C-C-0.536600         0    -14.43364   3.13505   8.1449   L
O-O--0.581900        0    -15.57068   2.64505   8.18881  L
C-CT--0.030300       0    -12.91022   1.60176   9.3949   L
C-C-0.799400         0    -12.21177   0.23677   9.38559  L
O-O2--0.801400       0    -12.7397  -0.68387   8.72158  L
O-O2--0.801400       0    -11.19871   0.03337   10.08517  L
H-H-0.293600         0    -11.17558   2.78027   8.04038  L
H-H1-0.088000        0    -13.55723   1.35629   7.3415   L
H-HC--0.012200       0    -13.84079   1.47555   9.95022  L
H-HC--0.012200       0    -12.31152   2.32518   9.9491   L
N-N--0.415700        0    -14.18952   4.44454   8.32722  L
C-CT--0.149000       -1   -15.13706   5.49154   8.73908  L
H-H-0.271900         0    -13.23422   4.74113   8.14424  L
H-H1-0.097600        0    -16.04101   5.42549   8.13143  L
H-H1-0.097600        0    -14.67999   6.47211   8.59536  L
H-H1-0.097600        0    -15.39888   5.36097   9.78948  L
C-CT--0.366200       -1   -19.80641  -1.08956  -1.34956  L
C-C-0.597200         0    -18.80098  -0.73599  -0.24241  L
O-O--0.567900        0    -18.39674   0.41804  -0.17874  L
H-HC-0.112300        0    -20.67054  -1.58561  -0.9145   L
H-HC-0.112300        0    -19.31815  -1.73859  -2.07503  L
H-HC-0.112300        0    -20.11884  -0.17205  -1.84659  L
N-N--0.415700        0    -18.38394  -1.67542   0.63548  L
C-CT--0.058100       -1   -17.25914  -1.455     1.59402  L
C-C-0.597300         0    -16.41734  -2.68777   1.93717  L
O-O--0.567900        0    -16.84573  -3.50461   2.75711  L
C-CT--0.007400       0    -17.69776  -0.67322   2.84342  L
C-CC-0.186800        0    -16.51138   0.05433   3.43338  L
N-NB--0.543200       0    -15.47228  -0.56168   4.12221  L
C-CW--0.220700       0    -16.18043   1.36386   3.22978  L
C-CR-0.163500        0    -14.51202   0.367     4.27622  L
N-NA--0.279500       0    -14.93084   1.54693   3.79445  L
H-H-0.271900         0    -18.75222  -2.60837   0.54032  L
H-H1-0.136000        0    -16.59914  -0.75501   1.08734  L
H-HC-0.036700        0    -18.12929  -1.34764   3.58341  L
H-HC-0.036700        0    -18.45046   0.06669   2.56936  L
H-H4-0.186200        0    -16.75251   2.08416   2.65901  L
H-H-0.333900         0    -14.35984   2.39028   3.82551  L
H-H5-0.143500        0    -13.54387   0.19981   4.73473  L
N-N--0.254800        0    -15.21296  -2.822     1.35104  L
C-CT--0.026600       -1   -14.26248  -3.83926   1.76687  L
C-C-0.589600         0    -13.57196  -3.50649   3.07977  L
O-O--0.574800        0    -13.17172  -2.36597   3.31435  L
C-CT--0.007000       0    -13.21476  -3.89006   0.66369  L
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C-CT-0.018900        0    -13.23684  -2.50047   0.02963  L
C-CT-0.019200        0    -14.67955  -2.04837   0.22851  L
H-H1-0.064100        0    -14.75636  -4.80844   1.84783  L
H-HC-0.025300        0    -13.54265  -4.62874  -0.05149  L
H-HC-0.025300        0    -12.22409  -4.14973   1.0401   L
H-HC-0.021300        0    -12.96449  -2.52672  -1.02585  L
H-HC-0.021300        0    -12.57153  -1.83061   0.57231  L
H-H1-0.039100        0    -14.68409  -0.97727   0.43212  L
H-H1-0.039100        0    -15.25757  -2.26631  -0.67106  L
N-N--0.347900        0    -13.30852  -4.52243   3.90338  L
C-CT--0.263700      -1    -12.54608  -4.34097   5.14538  L
C-C-0.734100         0    -11.03683  -4.68705   4.97491  L
O-O--0.589400        0    -10.71223  -5.54157   4.15631  L
C-CT--0.000700       0    -13.27354  -4.98634   6.33779  L
C-CT-0.039000        0    -14.59201  -4.23702   6.65968  L
C-CT-0.048600        0    -14.37929  -2.85231   7.3109   L
N-N2--0.529500       0    -15.2918  -1.80882   6.78668  L
C-CA-0.807600        0    -15.70125  -0.70658   7.40029  L
N-N2--0.862700       0    -15.41644  -0.43268   8.63296  L
N-N2--0.862700       0    -16.37188   0.21158   6.77342  L
H-H-0.274700         0    -13.58075  -5.44965   3.60208  L
H-H1-0.156000        0    -12.52032  -3.27511   5.36297  L
H-HC-0.032700        0    -12.62788  -4.96848   7.21776  L
H-HC-0.032700        0    -13.49825  -6.02637   6.09789  L
H-HC-0.028500        0    -15.1791  -4.8465    7.34734  L
H-HC-0.028500        0    -15.17798  -4.12817   5.74585  L
H-H1-0.068700        0    -13.35754  -2.52235   7.1292   L
H-H1-0.068700        0    -14.49886  -2.95489   8.39098  L
H-H-0.345600         0    -15.48486  -1.82336   5.7903   L
H-H-0.447800         0    -15.64474   0.49109   8.95559  L
H-H-0.447800         0    -14.52924  -0.85254   8.91203  L
H-H-0.447800         0    -16.44926   1.12707   7.19985  L
H-H-0.447800         0    -16.4096   0.11949   5.76518  L
N-N--0.415700        0    -10.11001  -3.97588   5.64882  L
C-CT--0.003100      -1    -8.624    -4.0869    5.53345  L
C-C-0.597300         0    -8.03119  -4.9204    6.67653  L
O-O--0.567900        0    -8.48758  -4.83446   7.81826  L
C-CT--0.003600       0    -7.98726  -2.69014   5.49086  L
C-CT--0.064500       0    -6.45178  -2.76713   5.41102  L
C-C-0.695100         0    -5.85614  -1.44016   4.99289  L
O-O--0.608600        0    -6.09716  -0.99507   3.8838   L
N-N--0.940700        0    -5.05727  -0.79471   5.80939  L
H-H-0.271900         0    -10.45377  -3.29013   6.31143  L
H-H1-0.085000        0    -8.40004  -4.6       4.60456  L
H-HC-0.017100        0    -8.2746   -2.12239   6.37422  L
H-HC-0.017100        0    -8.36937  -2.15726   4.62226  L
H-HC-0.035200        0    -6.15787  -3.50614   4.66658  L
H-HC-0.035200        0    -6.04821  -3.06614   6.37602  L
H-H-0.425100         0    -4.78777   0.156     5.58864  L
H-H-0.425100         0    -4.73493  -1.27411   6.66112  L
N-N--0.415700        0    -6.97795  -5.67991   6.37036  L
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C-CT--0.001400       -1   -6.23538  -6.5036    7.31937  L
C-C-0.597300         0    -4.73154  -6.44641   7.02946  L
O-O--0.567900        0    -4.29052  -6.61284   5.88626  L
C-CT--0.015200       0    -6.72092  -7.96484   7.25885  L
C-CA--0.001100       0    -8.21883  -8.14715   7.09452  L
C-CA--0.190600       0    -9.06515  -8.30747   8.21096  L
C-CA--0.190600       0    -8.76595  -8.10371   5.79916  L
C-CA--0.234100       0    -10.4584  -8.43871   8.02681  L
C-CA--0.234100       0    -10.15229  -8.20921   5.621    L
C-C-0.322600         0    -11.00255  -8.3933    6.72536  L
O-OH--0.557900       0    -12.33663  -8.53111   6.51354  L
H-H-0.271900         0    -6.6914   -5.72344   5.39687  L
H-H1-0.087600        0    -6.40942  -6.12314   8.32707  L
H-HC-0.029500        0    -6.3914   -8.47964   8.162    L
H-HC-0.029500        0    -6.23708  -8.45894   6.41453  L
H-HA-0.169900        0    -8.64732  -8.31511   9.20715  L
H-HA-0.169900        0    -8.12494  -7.94525   4.94146  L
H-HA-0.165600        0    -11.12324  -8.56271   8.86694  L
H-HA-0.165600        0    -10.57416  -8.11566   4.6384   L
H-HO-0.399200        0    -12.47734  -8.63934   5.56055  L
N-N--0.516300        0    -3.93029  -6.2245    8.06886  L
C-CT-0.039700        -1   -2.47929  -6.1508    7.94281  L
C-C-0.536600         0    -1.7941   -7.52571   8.02276  L
O-O--0.581900        0    -2.02305  -8.30859   8.94455  L
C-CT-0.056000        0    -1.86258  -5.16778   8.9457   L
C-CT-0.013600        0    -2.116    -3.7114    8.52903  L
C-C-0.805400         0    -3.59411  -3.29416   8.61933  L
O-O2--0.818800       0    -4.29448  -3.76593   9.54818  L
O-O2--0.818800       0    -4.03526  -2.49294   7.76648  L
H-H-0.293600         0    -4.34183  -5.92962   8.94627  L
H-H1-0.110500        0    -2.26784  -5.75365   6.9565   L
H-HC--0.017300       0    -0.78146  -5.31874   8.95541  L
H-HC--0.017300       0    -2.23768  -5.35799   9.95231  L
H-HC--0.042500       0    -1.75505  -3.57418   7.50757  L
H-HC--0.042500       0    -1.50812  -3.07096   9.16801  L
N-N--0.415700        0    -0.90321  -7.8102    7.06656  L
C-CT--0.002400       -1   -0.14903  -9.06692   6.96571  L
C-C-0.597300         0     1.35443  -8.83861   7.14318  L
O-O--0.567900        0     1.87569  -7.7189    7.16737  L
C-CT--0.034300       0    -0.49467  -9.75309   5.62473  L
C-CA-0.011800        0     0.07116  -9.07308   4.38553  L
C-CA--0.125600       0    -0.64533  -8.05264   3.73504  L
C-CA--0.125600       0     1.34103  -9.43509   3.90108  L
C-CA--0.170400       0    -0.06338  -7.35259   2.66118  L
C-CA--0.170400       0     1.92665  -8.73478   2.83088  L
C-CA--0.107200       0     1.22414  -7.68743   2.21317  L
H-H-0.271900         0    -0.76465  -7.10725   6.3455   L
H-H1-0.097800        0    -0.4749   -9.72996   7.76801  L
H-HC-0.029500        0    -1.58064  -9.81164   5.53036  L
H-HC-0.029500        0    -0.12685  -10.77906   5.65379  L
H-HA-0.133000        0    -1.62559  -7.76725   4.09304  L
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H-HA-0.133000        0     1.87243  -10.24674   4.36714  L
H-HA-0.143000        0    -0.58926  -6.52803   2.20113  L
H-HA-0.143000        0     2.91543  -8.99474   2.48639  L
H-HA-0.129700        0     1.66847  -7.12726   1.40343  L
N-N--0.415700        0     2.08146  -9.94384   7.28984  L
C-CT--0.024900       -1    3.52499  -9.90293   7.48072  L
C-C-0.597300         0     4.27878  -9.42065   6.22424  L
O-O--0.567900        0     4.15321  -9.98846   5.14161  L
C-CT-0.211700        0     4.06042  -11.27987   7.91326  L
O-OH--0.654600       0     3.80599  -12.30929   6.9635   L
H-H-0.271900         0     1.59852  -10.82441   7.22554  L
H-H1-0.084300        0     3.73524  -9.2029    8.29026  L
H-H1-0.035200        0     3.60541  -11.55411   8.86662  L
H-H1-0.035200        0     5.13828  -11.20209   8.06509  L
H-HO-0.427500        0     3.06988  -12.83926   7.29587  L
N-N--0.347900        0     5.13544  -8.40581   6.36582  L
C-CT--0.263700       -1    6.03492  -7.88892   5.30976  L
C-C-0.734100         0     7.11143  -8.89626   4.86848  L
O-O--0.589400        0     7.15702  -10.03749   5.33315  L
C-CT--0.000700       0     6.61047  -6.55411   5.83292  L
C-CT-0.039000        0     7.7219   -6.69793   6.8895   L
C-CT-0.048600        0     8.07256  -5.36977   7.57587  L
N-N2--0.529500       0     8.38951  -4.28675   6.6201   L
C-CA-0.807600        0     7.62635  -3.25668   6.29711  L
N-N2--0.862700       0     6.41725  -3.14511   6.75389  L
N-N2--0.862700       0     8.04776  -2.30206   5.52556  L
H-H-0.274700         0     5.12601  -7.95396   7.26671  L
H-H1-0.156000        0     5.4222   -7.67378   4.4315   L
H-HC-0.032700        0     5.79147  -5.96515   6.25031  L
H-HC-0.032700        0     7.01199  -5.98523   5.00308  L
H-HC-0.028500        0     8.62069  -7.08813   6.41526  L
H-HC-0.028500        0     7.40747  -7.40472   7.65799  L
H-H1-0.068700        0     8.94161  -5.53581   8.21504  L
H-H1-0.068700        0     7.24665  -5.07856   8.22628  L
H-H-0.345600         0     9.32117  -4.28762   6.21241  L
H-H-0.447800         0     5.86294  -2.31597   6.50337  L
H-H-0.447800         0     6.02118  -3.81018   7.37629  L
H-H-0.447800         0     7.3768   -1.5424    5.38933  L
H-H-0.447800         0     8.94087  -2.3096    5.06075  L
N-N--0.415700        0     7.99811  -8.45246   3.98622  L
C-CT--0.051800       -1    9.32693  -9.00018   3.717    L
C-C-0.597300         0     10.27169  -7.8104    3.87679  L
O-O--0.567900        0     10.36633  -6.94675   3.01017  L
C-CT--0.110200       0     9.32611  -9.64258   2.31338  L
C-CT-0.353100        0     10.63126  -10.34141   1.87745  L
C-CT--0.412100       0     10.3111  -11.37559   0.79505  L
C-CT--0.412100       0     11.66639  -9.39169   1.27602  L
H-H-0.271900         0     7.82146  -7.53461   3.58553  L
H-H1-0.092200        0     9.58269  -9.7631    4.4548   L
H-HC-0.045700        0     9.04377  -8.90261   1.5632   L
H-HC-0.045700        0     8.54639  -10.39767   2.32674  L
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H-HC--0.036100       0     11.06691  -10.85904   2.73222  L
H-HC-0.100000        0     11.22547  -11.88544   0.48982  L
H-HC-0.100000        0     9.87509   -10.8816  -0.07553  L
H-HC-0.100000        0     9.61571   -12.12063   1.17842  L
H-HC-0.100000        0     12.53041  -9.95856    0.93043  L
H-HC-0.100000        0     12.00642  -8.67529    2.01533  L
H-HC-0.100000        0     11.23316  -8.85351    0.43387  L
N-N--0.415700        0     10.9248   -7.71918    5.02914  L
C-CT-0.014300        -1    12.21623  -7.05848    5.0631   L
C-C-0.597300         0     13.24115  -8.13212    4.60889  L
O-O--0.567900        0     13.21791  -9.22325    5.17875  L
C-CT--0.204100       0     12.5701   -6.58453    6.48381  L
C-C-0.713000         0     11.80545  -5.3661     6.9585   L
O-O--0.593100        0     11.1248   -4.66866    6.22282  L
N-N--0.919100        0     11.89355  -5.06212    8.23145  L
H-H-0.271900         0     10.81712  -8.4867     5.6746   L
H-H1-0.104800        0     12.25286  -6.21481    4.37205  L
H-HC-0.079700        0     13.62981  -6.32483    6.50107  L
H-HC-0.079700        0     12.41759  -7.40346    7.18717  L
H-H-0.419600         0     11.43802  -4.21848    8.52415  L
H-H-0.419600         0     12.49754  -5.59634    8.83509  L
N-N--0.415700        0     14.08203  -7.88861    3.5924   L
C-CT--0.051800       -1    15.18219  -8.80504    3.23316  L
C-C-0.597300         0     16.39644  -8.58183    4.17285  L
O-O--0.567900        0     16.66982  -7.44212    4.54574  L
C-CT--0.110200       0     15.55017  -8.67036    1.72141  L
C-CT-0.353100        0     16.56996  -9.70275    1.15474  L
C-CT--0.412100       0     16.07615  -11.14116   1.34846  L
C-CT--0.412100       -1    16.85562  -9.55003  -0.35958  L
H-H-0.271900         0     14.06237  -6.99057    3.13248  L
H-H1-0.092200        0     14.82832  -9.82165    3.40073  L
H-HC-0.045700        0     15.95244  -7.67241    1.55135  L
H-HC-0.045700        0     14.63409  -8.75183    1.13748  L
H-HC--0.036100       0     17.51257  -9.58906    1.6854   L
H-HC-0.100000        0     15.10071  -11.26927   0.87972  L
H-HC-0.100000        0     16.00863  -11.38218   2.40678  L
H-HC-0.100000        0     16.78576  -11.83457   0.89612  L
H-HC-0.100000        0     15.96002  -9.77226  -0.93582  L
H-HC-0.100000        0     17.65581  -10.22987 -0.65238  L
H-HC-0.100000        0     17.1813   -8.52838  -0.55883  L
N-N--0.516300        0     17.11828  -9.64134    4.57103  L
C-CT-0.039700        -1    18.3708   -9.51496    5.3551   L
C-C-0.536600         0     19.45859  -8.71652    4.57888  L
O-O--0.581900        0     19.39248  -8.59218    3.35271  L
C-CT-0.056000        0     18.89703  -10.88407   5.82723  L
C-CT-0.013600        0     18.59009  -11.1319    7.31442  L
C-C-0.805400         0     19.11983  -10.01993   8.24212  L
O-O2--0.818800       0     18.5356   -9.8605     9.33414  L
O-O2--0.818800       0     20.04668  -9.28665    7.81837  L
H-H-0.293600         0     16.86119  -10.5562    4.24502  L
H-H1-0.110500        0     18.13479  -8.90206    6.22566  L
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H-HC--0.017300       0     19.97778  -10.9328   5.68596  L
H-HC--0.017300       0     18.45371  -11.68156   5.22813  L
H-HC--0.042500       0     19.03221  -12.08741   7.60517  L
H-HC--0.042500       0     17.50636  -11.21652   7.42794  L
N-N--0.415700        0     20.42539  -8.09895   5.27624  L
C-CT--0.025200       -1    21.43495  -7.16774   4.70983  L
C-C-0.597300         0     20.82257  -5.89722   4.05337  L
O-O--0.567900        0     21.57254  -5.1272    3.45727  L
H-H-0.271900         0     20.44388  -8.31314   6.27792  L
H-H1-0.069800        0     22.01595  -7.69175   3.95106  L
H-H1-0.069800        0     22.11155  -6.84987   5.50225  L
N-N--0.415700        0     19.49686  -5.64478   4.12893  L
C-CT--0.038900       0     18.7691  -4.74056   3.19759  L
C-C-0.597300         0     17.80227  -3.73398   3.86595  L
O-O--0.567900        0     16.96817  -4.07645   4.70142  L
C-CT-0.365400        0     17.97727  -5.56219   2.15802  L
O-OH--0.676100       0     18.74954  -6.58954   1.57859  L
C-CT--0.243800       0     17.51995  -4.71489   0.96901  L
H-H-0.271900         0     18.937   -6.30534   4.65299  L
H-H1-0.100700        0     19.50969  -4.16654   2.64217  L
H-H1-0.004300        0     17.10007  -5.99736   2.63012  L
H-HC-0.064200        0     16.86577  -3.91116   1.29683  L
H-HC-0.064200        0     16.97144  -5.3469    0.27034  L
H-HC-0.064200        0     18.38738  -4.29511   0.45895  L
H-HO-0.410200        0     18.97507  -7.24681   2.26434  L
N-N--0.415700        0     17.85338  -2.46212   3.44258  L
C-CT--0.087500       -1    16.94842  -1.35259   3.8423   L
C-C-0.597300         0     15.58387  -1.48177   3.12808  L
O-O--0.567900        0     15.53421  -1.48024   1.90138  L
C-CT-0.298500        0     17.54992   0.01532   3.43291  L
C-CT--0.319200       -1    16.68352   1.22182   3.89636  L
C-CT--0.319200       -1    18.99415   0.11007   3.95505  L
H-H-0.271900         0     18.54572  -2.26195   2.73637  L
H-H1-0.096900        0     16.80443  -1.37635   4.92192  L
H-HC--0.029700       0     17.61117   0.06168   2.34523  L
H-HC-0.079100        0     16.56662   1.20288   4.97919  L
H-HC-0.079100        0     15.70756   1.20011   3.41239  L
H-HC-0.079100        0     17.18221   2.14903   3.61083  L
H-HC-0.079100        0     19.01743  -0.06071   5.03162  L
H-HC-0.079100        0     19.38811   1.10555   3.74796  L
H-HC-0.079100        0     19.64285  -0.61004   3.45685  L
N-N--0.415700        0     14.46223  -1.59218   3.85908  L
C-CT--0.023700       -1    13.15875  -2.01825   3.28371  L
C-C-0.597300         0     11.89082  -1.37368   3.92287  L
O-O--0.567900        0     10.78191  -1.91859   3.86326  L
C-CT-0.034200        0     13.04399  -3.55047   3.50372  L
C-CT-0.001800        0     14.13304  -4.46218   2.91453  L
S-S--0.273700        0     13.66931  -5.34612   1.40195  L
C-CT--0.053600       0     13.81791  -3.99876   0.20401  L
H-H-0.271900         0     14.60427  -1.68493   4.85274  L
H-H1-0.088000        0     13.12784  -1.81175   2.21322  L
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 H-HC-0.024100        0     12.08657  -3.90508   3.11941  L
 H-HC-0.024100        0     13.03738  -3.7209    4.58075  L
 H-H1-0.044000        0     14.3746  -5.2096    3.66941  L
 H-H1-0.044000        0     15.04983  -3.91259   2.73047  L
 H-H1-0.068400        0     14.82583  -3.58531   0.23017  L
 H-H1-0.068400        0     13.10278  -3.21231   0.43932  L
 H-H1-0.068400        0     13.61499  -4.38723  -0.79139  L
 N-N--0.415700        0     12.02524  -0.19459   4.53342  L
 C-CT--0.024900       -1    10.91475   0.72669   4.85714  L
 C-C-0.597300         0     11.01566   1.84038   3.82049  L
 O-O--0.567900        0     12.10671   2.37246   3.61983  L
 C-CT-0.211700        0     11.05718   1.20829   6.29722  L
 O-OH--0.654600       0     10.14418   2.23153   6.65036  L
 H-H-0.271900         0     12.94457   0.21776   4.45964  L
 H-H1-0.084300        0     9.95273   0.22453   4.74828  L
 H-H1-0.035200        0     12.0691   1.57781   6.41946  L
 H-H1-0.035200        0     10.91421   0.35807   6.96588  L
 H-HO-0.427500        0     9.25287   1.97731   6.30503  L
 N-N--0.347900        0     9.93819   2.12574   3.08103  L
 C-CT--0.240000       -1    9.97873   3.03446   1.9204   L
 C-C-0.734100         0     10.53286   4.41909   2.3396   L
 O-O--0.589400        0     11.55373   4.81039   1.78101  L
 C-CT--0.009400       0     8.59919   3.05136   1.25081  L    H-HC
1447  0.        0.
 C-CT-0.018700        0     8.54983   3.88049  -0.03967  H
 C-CT--0.047900       0     7.49146   3.34716  -1.00307  H
 C-CT--0.014300       0     7.33089   4.21212  -2.23733  H
 N-N3--0.385400       0     6.46254   3.54658  -3.22091  H
 H-H-0.274700         0     9.07408   1.64614   3.30778  L
 H-H1-0.142600        0     10.69276   2.63201   1.19932  L
 H-HC-0.036200        0     7.85763   3.42829   1.94897  L
 H-HC-0.036200        0     8.33457   2.01876   1.01257  L
 H-HC-0.010300        0     9.53219   3.84518  -0.52256  H
 H-HC-0.010300        0     8.35162   4.92387   0.23246  H
 H-HC-0.062100        0     6.50795   3.25525  -0.53323  H
 H-HC-0.062100        0     7.76295   2.33955  -1.34317  H
 H-HP-0.113500        0     8.30902   4.47093  -2.66534  H
 H-HP-0.113500        0     6.85265   5.16727  -1.98157  H
 H-H-0.340000         0     7.00415   3.05725  -3.93556  H
 H-H-0.340000         0     6.04527   4.27656  -3.8307   H
 H-H-0.340000         0     3.51255   2.78805  -0.88258  H
 N-N--0.347900        0     10.00962   5.07913   3.40018  L
 C-CT--0.263700       -1    10.63806   6.23158   4.13788  L
 C-C-0.734100         0     11.79617   5.81248   5.0248   L
 O-O--0.589400        0     11.80848   6.09777   6.22405  L
 C-CT--0.000700       0     9.55015   7.06543   4.85428  L
 C-CT-0.039000        0     8.62941   7.76524   3.83376  L
 C-CT-0.048600        0     7.56391   8.69116   4.44191  L
 N-N2--0.529500       0     6.65939   8.02176   5.3981   L
 C-CA-0.807600        0     5.45251   8.42428   5.75913  L
 N-N2--0.862700       0     4.81661   9.39609   5.1795   L
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N-N2--0.862700       0     4.84802   7.84375   6.74696  L
H-H-0.274700         0     9.13387   4.70874   3.75302  L
H-H1-0.156000        0     11.09783   6.89156   3.39608  L
H-HC-0.032700        0     10.02752   7.8376    5.46017  L
H-HC-0.032700        0     8.96608   6.41852   5.50973  L
H-HC-0.028500        0     8.13471   7.02096   3.21551  L
H-HC-0.028500        0     9.24805   8.37201   3.1713   L
H-H1-0.068700        0     6.97719   9.0985    3.61713  L
H-H1-0.068700        0     8.06223   9.52158   4.94536  L
H-H-0.345600         0     6.97982   7.20868   5.90633  L
H-H-0.447800         0     3.85573   9.59613   5.46384  L
H-H-0.447800         0     5.13198   9.80502   4.32402  L
H-H-0.447800         0     3.93363   8.22041   7.0009   L
H-H-0.447800         0     5.23951   7.04272   7.21076  L
N-N--0.347900        0     12.73343   5.11775   4.37014  L
C-CT--0.240000       -1    14.12214   4.76208   4.70428  L
C-C-0.734100         0     14.97917   4.48696   3.43634  L
O-O--0.589400        0     16.18783   4.66684   3.4976   L
C-CT--0.009400       0     14.29348   3.60452   5.72665  L
C-CT-0.018700        0     13.47512   3.90612   6.98003  L
C-CT--0.047900       0     13.57187   3.04471   8.24257  L
C-CT--0.014300       0     12.58614   3.57607   9.31424  L
N-N3--0.385400       0     11.2449   3.96354   8.77538  L
H-H-0.274700         0     12.47586   5.02643   3.39477  L
H-H1-0.142600        0     14.57927   5.6478    5.15011  L
H-HC-0.036200        0     15.34744   3.52824   5.9995   L
H-HC-0.036200        0     13.9795   2.65604   5.29366  L
H-HC-0.010300        0     12.4505   3.81949   6.63744  L
H-HC-0.010300        0     13.69945   4.92893   7.28603  L
H-HC-0.062100        0     14.589    3.09182   8.63588  L
H-HC-0.062100        0     13.34774   2.00464   8.01502  L
H-HP-0.113500        0     13.04254   4.45409   9.78198  L
H-HP-0.113500        0     12.47493   2.81289   10.09003  L
H-H-0.340000         0     11.34251   4.74353   8.1274   L
H-H-0.340000         0     10.60479   4.239     9.50738  L
H-H-0.340000         0     10.82343   3.21109   8.23115  L
N-N--0.415700        0     14.38714   4.04115   2.31497  L
C-CT--0.051800       -1    15.04654   3.63169   1.04522  L
C-C-0.597300         0     15.27571   4.73332   0.04673  L
O-O--0.567900        0     16.24614   4.70136  -0.70685  L
C-CT--0.110200       0     14.19558   2.48259   0.46143  L
C-CT-0.353100        0     14.74278   1.8108   -0.81375  L
C-CT--0.412100       0     16.12629   1.19331  -0.60653  L
C-CT--0.412100       0     13.78674   0.69334  -1.24031  L
H-H-0.271900         0     13.39136   3.8797    2.37738  L
H-H1-0.092200        0     16.03124   3.23418   1.29665  L
H-HC-0.045700        0     13.20058   2.87193   0.23977  L
H-HC-0.045700        0     14.08714   1.71382   1.22875  L
H-HC--0.036100       0     14.79309   2.54207  -1.61977  L
H-HC-0.100000        0     16.10526   0.48757   0.22308  L
H-HC-0.100000        0     16.85793   1.9747   -0.40328  L
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H-HC-0.100000        0     16.43536   0.67145  -1.51193  L
H-HC-0.100000        0     14.14175   0.24667  -2.16905  L
H-HC-0.100000        0     12.79026   1.10073  -1.40749  L
H-HC-0.100000        0     13.7414  -0.07692  -0.46907  L
N-N--0.415700        0     14.37769   5.70227   0.03821  L
C-CT-0.014300        -1    14.5809    6.90543  -0.72395  L
C-C-0.597300         0     15.66156   7.83554  -0.09848  L
O-O--0.567900        0     15.36468   8.93351   0.36591  L
C-CT--0.204100       0     13.21335   7.58546  -0.99089  L
C-C-0.713000         0     12.25694   7.72005   0.19225  L
O-O--0.593100        0     12.58466   7.56718   1.35982  L
N-N--0.919100        0     10.99358   7.96122  -0.07963  L
H-H-0.271900         0     13.62867   5.68807   0.7195   L
H-H1-0.104800        0     14.97621   6.62859  -1.70317  L
H-HC-0.079700        0     12.69876   7.00385  -1.7549   L
H-HC-0.079700        0     13.3869    8.58131  -1.39748  L
H-H-0.419600         0     10.39839   8.02411   0.72005  L
H-H-0.419600         0     10.63708   8.05951  -1.02776  L
N-N--0.415700        0     16.93186   7.39646  -0.13686  L
C-CT--0.149000       -1    18.12814   8.08437   0.36503  L
H-H-0.271900         0     17.04414   6.46     -0.51213  L
H-H1-0.097600        0     18.11658   8.08735   1.45633  L
H-H1-0.097600        0     18.13438   9.11715   0.01116  L
H-H1-0.097600        0     19.02746   7.57631   0.01449  L
C-CT--0.055800       0     1.27964   14.76919   4.43243  L
C-CT-0.000000        0     1.55747   13.88598   3.21716  L
O-OS--0.354800       0     2.94575   13.90471   2.90915  L
C-CT--0.202200       0     1.20169   12.42631   3.50734  L
O-OS--0.524600       0     0.63666   11.88753   2.31121  L
C-CT--0.067000       0     2.56228   11.83002   3.84454  L
O-OH--0.613900       0     2.58356   10.43523   3.67773  L
C-CT--0.006600       0     3.34435   12.55339   2.76884  L
N-N*--0.048400       0     4.80748   12.34251   2.87519  L
C-C-0.753800         0     5.41916   11.47725   1.96397  L
O-O--0.625200        0     4.77153   10.89571   1.09578  L
N-NC--0.758400       0     6.7607    11.2704    2.01107  L
C-CA-0.818500        0     7.45736   11.90225   2.92814  L
N-N2--0.953000       0     8.73998   11.68112   2.89521  L
C-CM--0.521500       0     6.88914   12.74786   3.91579  L
C-CM--0.005300       0     5.54783   12.94853   3.85819  L
H-H1-0.067900        0     0.20738   14.77417   4.63173  L
H-H1-0.067900        0     1.80184   14.36838   5.30116  L
H-H1-0.117400        0     0.9574    14.2397    2.37465  L
H-H1-0.061500        0     0.49477   12.36472   4.33355  L
H-H1-0.097200        0     2.8814    12.13018   4.84503  L
H-HO-0.418600        0     1.83229   10.23768   3.09112  L
H-H2-0.202900        0     2.97433   12.17304   1.81447  L
H-H-0.423400         0     9.04128   11.15301   2.09868  L
H-H-0.423400         0     9.3501    12.2064    3.49064  L
H-HA-0.192800        0     7.47155   13.24305   4.6752   L
H-H4-0.195800        0     5.04364   13.59585   4.5682   L
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```
 P-P-1.166200          0    -0.36244   10.62004   2.28015  L
 O-O2--0.776000        0    -1.3769    10.80929   1.22474  L
 O-O2--0.776000        0    -0.76121   10.26412   3.65964  L
 O-OS--0.498900        0     0.63094   9.45505   1.80585  L
 C-CT-0.055800         0     1.38114   9.55278   0.60904  L    H-H1
1581  0.        0.
 C-CT-0.106500         0     2.1157    8.23027   0.33231  H
 O-OS--0.354800        0     2.9205    7.8984    1.46513  H
 C-CT-0.202200         0     1.16813   7.05097   0.04145  H
 O-OH--0.654100        0     1.40958   6.42671  -1.2023   H
 C-CT-0.067000         0     1.4732    6.00903   1.15888  H
 O-OH--0.613900        0     1.96508   4.76475   0.68101  H
 C-CT-0.039400         0     2.64563   6.60548   1.95135  H
 N-N*--0.025100        0     2.4447    6.62915   3.37764  H
 C-CK-0.200600         0     1.53576   7.33856   4.15006  H
 N-NB--0.607300        0     1.55274   6.99487   5.40937  H
 C-CB-0.051500         0     2.49056   5.98848   5.48266  H
 C-CA-0.700900         0     2.90819   5.14234   6.52867  H
 N-N2--0.901900        0     2.44626   5.27442   7.80251  H
 N-NC--0.761500        0     3.88388   4.25131   6.28114  H
 C-CQ-0.587500         0     4.26834   4.07731   5.01737  H
 N-NC--0.699700        0     3.96092   4.80861   3.95229  H
 C-CB-0.305300         0     3.05703   5.74844   4.23641  H
 H-H1-0.067900         0     2.11091   10.3558   0.70771  L
 H-H1-0.067900         0     0.71502   9.77945  -0.22658  L
 H-H1-0.117400         0     2.76167   8.37067  -0.54259  H
 H-H1-0.061500         0     0.12063   7.37017   0.11031  H
 H-HO-0.437600         0     1.02072   6.95932  -1.93651  H
 H-H1-0.097200         0     0.59448   5.87906   1.79899  H
 H-HO-0.418600         0     5.04166   4.14568   0.88428  H
 H-H2-0.200700         0     3.49732   5.95613   1.76789  H
 H-H5-0.155300         0     0.89953   8.10325   3.72014  H
 H-H-0.411500          0     2.40412   4.3847    8.31531  H
 H-H-0.411500          0     1.54917   5.75051   7.86671  H
 H-H5-0.047300         0     4.98036   3.27977   4.83825  H
 N-N3-0.149300         0    -0.99114   4.8782   -0.29603  H
 C-CT-0.053600         0    -0.32537   3.82566   0.50958  H
 C-CT-0.065100         0    -0.95041   2.44855   0.26359  H
 C-CT--0.090300        0    -0.65935   1.42077   1.36654  H
 C-C-0.735400          0    -1.59328   0.21755   1.2595   H
 O-O--0.613300         0    -1.22093  -0.90665   0.99015  H
 N-N--1.003100         0    -2.93761   0.52889   1.38863  H
 C-C-0.612300          0     1.14631   3.83289   0.11438  H
 O-O--0.571300         0     1.61968   3.0363   -0.64894  H
 O-OS--0.421200        0     2.70513   1.43999   1.2825   H
 P-P-1.166200          0     3.99854   1.26104   0.60028  H
 O-O2--0.776000        0     5.31968   1.31022   1.4699   H
 O-O2--0.776000        0     4.3158    2.34466  -0.53892  H
 O-OS--0.498900        0     4.20077  -0.15312  -0.10951  H
 C-CT-0.055800         0     3.28418  -0.49521  -1.16858  H
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 C-CT-0.106500        0     2.62868  -1.86598  -0.91833  L    H-H1
1624  0.        0.
 O-OS--0.354800       0     3.55942  -2.86399  -0.48614  L
 C-CT-0.039400        0     3.39017  -3.07301   0.91902  L
 N-N*--0.025100       0     4.71288  -3.04937   1.59561  L
 C-CB-0.305300        0     5.47519  -4.16063   1.8508   L
 N-NC--0.699700       0     5.12661  -5.45813   1.62712  L
 C-CQ-0.587500        0     6.08553  -6.29503   1.98336  L
 N-NC--0.761500       0     7.27945  -6.01393   2.48934  L
 C-CA-0.700900        0     7.5942   -4.72937   2.65087  L
 N-N2--0.901900       0     8.82644  -4.54069   3.08656  L
 C-CB-0.051500        0     6.66406  -3.70731   2.35878  L
 N-NB--0.607300       0     6.66795  -2.3146    2.47474  L
 C-CK-0.200600        0     5.46961  -1.99129   2.05093  L
 C-CT-0.067000        0     2.36738  -2.05481   1.43131  L
 O-OH--0.613900       0     1.57139  -2.54371   2.49532  L
 C-CT-0.202200        0     1.5565   -1.80717   0.16019  L
 O-OH--0.654100       0     0.59661  -2.83708  -0.06382  L
 H-H-0.199600         0    -1.86239   3.94573  -1.65763  H
 H-H-0.199600         0    -0.32672   5.45155  -0.80777  H
 H-H-0.199600         0    -1.55978   5.48482   0.28865  H
 H-HP-0.101500        0    -0.39777   4.06902   1.57983  H
 H-HC-0.005000        0    -0.593     2.07315  -0.69703  H
 H-HC-0.005000        0    -2.02811   2.58549   0.15334  H
 H-HC-0.033100        0    -0.82628   1.88366   2.35032  H
 H-HC-0.033100        0     0.3761    1.07548   1.33083  H
 H-H-0.442900         0    -3.52606  -0.25837   1.62674  H
 H-H-0.442900         0    -3.13158   1.32783   2.00389  H
 H-H1-0.067900        0     3.84853  -0.53944  -2.10202  H
 H-H1-0.067900        0     2.49569   0.25217  -1.28215  H
 H-H1-0.117400        0     2.1485   -2.16443  -1.85066  L
 H-H2-0.200700        0     2.94211  -4.05717   1.0682   L
 H-H5-0.047300        0     5.86361  -7.34278   1.84579  L
 H-H-0.411500         0     9.19245  -3.60485   3.16199  L
 H-H-0.411500         0     9.42196  -5.3632    3.10204  L
 H-H5-0.155300        0     5.12016  -0.97213   2.02649  L
 H-H1-0.097200        0     2.85502  -1.13034   1.73026  L
 H-HO-0.418600        0     2.12796  -2.62577   3.29576  L
 H-H1-0.061500        0     1.08143  -0.82701   0.17788  L
 H-HO-0.437600        0    -0.18085  -2.53005   0.44147  L
 O-OW--0.834000       0    -10.34894  -2.02374   11.52952  L
 H-HW-0.417000        0    -10.64947  -1.18124   11.11267  L
 H-HW-0.417000        0    -10.63837  -2.68568   10.87686  L
 O-OW--0.834000       0    -10.32179  -3.80974   9.47464  L
 H-HW-0.417000        0    -10.58024  -3.17213   8.78231  L
 H-HW-0.417000        0    -9.6894   -4.38074   8.99747  L
 O-OW--0.834000       0    -10.76755  -1.90635   7.62311  L
 H-HW-0.417000        0    -11.57076  -1.50251   8.03997  L
 H-HW-0.417000        0    -10.12387  -1.19824   7.73468  L
 O-OW--0.834000       0     5.331     3.89195   1.78461  H
 H-HW-0.417000        0     4.61549   4.20601   2.39136  H
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H-HW-0.417000        0     5.42834   2.2769    1.70461  H
O-OW--0.834000       0     6.92497   4.86421   3.94609  H
H-HW-0.417000        0     6.67007   4.37328   3.14251  H
H-HW-0.417000        0     6.45195   5.69391   3.72913  H
O-OW--0.834000       0     6.36569   2.22253  -5.74075  L
H-HW-0.417000        0     7.2488    1.92799  -6.03125  L
H-HW-0.417000        0     6.2394    3.05254  -6.2175   L
O-OW--0.834000       0     6.56132   5.35603   6.65257  L
H-HW-0.417000        0     5.74591   4.87386   6.87704  L
H-HW-0.417000        0     6.73892   5.05929   5.74185  L
O-OW--0.834000       0     7.79498   1.57695   5.51457  H
H-HW-0.417000        0     7.11434   2.22456   5.27659  H
H-HW-0.417000        0     7.19487   0.8126    5.75378  H
O-OW--0.834000       0     5.69738   7.05062   2.18901  H
H-HW-0.417000        0     4.9598    7.68158   2.08507  H
H-HW-0.417000        0     5.48233   6.39373   1.49795  H
O-OW--0.834000       0     4.29279   16.03764   4.0097   L
H-HW-0.417000        0     3.77807   15.30879   3.62992  L
H-HW-0.417000        0     3.62677   16.68909   4.23219  L
O-OW--0.834000       0    -4.42961   2.18835   5.83192  L
H-HW-0.417000        0    -4.32026   2.123     6.78559  L
H-HW-0.417000        0    -4.87398   3.07494   5.73854  L
O-OW--0.834000       0     0.22912   1.92498   12.12589  L
H-HW-0.417000        0    -0.13999   1.66783   12.99315  L
H-HW-0.417000        0    -0.04837   2.84354   12.07258  L
O-OW--0.834000       0    -2.34684   9.99386   5.7891   L
H-HW-0.417000        0    -2.22246   9.09036   6.14716  L
H-HW-0.417000        0    -1.82499   9.99376   4.95506  L
O-OW--0.834000       0     2.39516   9.24117   6.78949  L
H-HW-0.417000        0     1.90031   8.49299   6.40389  L
H-HW-0.417000        0     1.72169   9.95542   6.73149  L
O-OW--0.834000       0    -4.94694   9.16183   5.46342  L
H-HW-0.417000        0    -4.86532   8.27753   5.87494  L
H-HW-0.417000        0    -4.0869    9.57414   5.65761  L
O-OW--0.834000       0    -2.43953   7.55214   7.0057   L
H-HW-0.417000        0    -3.28934   7.10891   6.77555  L
H-HW-0.417000        0    -2.22697   7.18001   7.87827  L
O-OW--0.834000       0     0.27749   10.78215   6.23434  L
H-HW-0.417000        0     0.24067   10.80273   5.26002  L
H-HW-0.417000        0    -0.6592    10.66226   6.45603  L
N-N                  0     5.54608   7.76879  -0.77097  H
H-H                  0     6.00086   7.85262   0.13279  H
H-H                  0     5.73867   8.45353  -1.48359  H
```

## ND-GluRS

**Table S1.** Cartesian coordinates and partial charges of all ND-GluRS species presently optimized using the ONIOM(QM/MM) approach.

**RC**

| | | | | | |
|---|---|---|---|---|---|
| H-HW-0.417000 | 0 | 2.54765 | -6.05309 | 4.64938 | L |
| H-HW-0.417000 | 0 | 3.2898 | -6.72895 | 5.8118 | L |
| O-OW--0.834000 | 0 | 4.99226 | -2.7124 | -3.77502 | L |
| H-HW-0.417000 | 0 | 4.07327 | -2.50986 | -4.01539 | L |
| H-HW-0.417000 | 0 | 5.05419 | -2.39318 | -2.8606 | L |
| O-OW--0.834000 | 0 | 0.72744 | -13.83248 | -3.36704 | L |
| H-HW-0.417000 | 0 | -0.18165 | -13.59991 | -3.6437 | L |
| H-HW-0.417000 | 0 | 1.22824 | -13.67387 | -4.18473 | L |
| O-OW--0.834000 | 0 | 4.34081 | -4.75209 | -1.52329 | L |
| H-HW-0.417000 | 0 | 4.77024 | -4.91403 | -2.38418 | L |
| H-HW-0.417000 | 0 | 3.63755 | -4.10513 | -1.75282 | L |
| O-OW--0.834000 | 0 | 2.67332 | -9.95448 | -0.88121 | L |
| H-HW-0.417000 | 0 | 2.30836 | -10.41359 | -1.66041 | L |
| H-HW-0.417000 | 0 | 2.38747 | -9.03609 | -1.03734 | L |
| O-OW--0.834000 | 0 | -0.17067 | -11.02238 | -7.72885 | L |
| H-HW-0.417000 | 0 | -0.18607 | -10.5321 | -6.84823 | L |
| H-HW-0.417000 | 0 | -0.65374 | -11.81936 | -7.50085 | L |
| O-OW--0.834000 | 0 | 7.50855 | -10.67514 | -0.30363 | L |
| H-HW-0.417000 | 0 | 7.30357 | -9.72843 | -0.26865 | L |
| H-HW-0.417000 | 0 | 6.75752 | -11.00935 | -0.83146 | L |
| O-OW--0.834000 | 0 | 3.94655 | -4.24152 | 1.10314 | L |
| H-HW-0.417000 | 0 | 3.00517 | -4.05159 | 0.91393 | L |
| H-HW-0.417000 | 0 | 4.25868 | -4.48259 | 0.20973 | L |
| O-OW--0.834000 | 0 | 2.40848 | -2.92485 | -2.13964 | H |
| H-HW-0.417000 | 0 | 1.48753 | -2.97906 | -1.83015 | H |
| H-HW-0.417000 | 0 | 2.26812 | -2.64747 | -3.07697 | H |
| O-OW--0.834000 | 0 | 8.95547 | -8.2111 | -4.14971 | L |
| H-HW-0.417000 | 0 | 8.00618 | -8.16057 | -3.90254 | L |
| H-HW-0.417000 | 0 | 9.20947 | -7.27059 | -4.20426 | L |
| O-OW--0.834000 | 0 | 4.35925 | -8.97601 | -6.72771 | L |
| H-HW-0.417000 | 0 | 3.74296 | -9.61623 | -7.13546 | L |
| H-HW-0.417000 | 0 | 4.33514 | -9.22386 | -5.78674 | L |
| O-OW--0.834000 | 0 | 1.39813 | -3.91875 | -8.30753 | L |
| H-HW-0.417000 | 0 | 1.25394 | -2.95106 | -8.362 | L |
| H-HW-0.417000 | 0 | 0.62001 | -4.27358 | -8.748 | L |
| O-OW--0.834000 | 0 | 2.62138 | -1.71399 | 4.20225 | H |
| H-HW-0.417000 | 0 | 1.84344 | -2.19086 | 3.86478 | H |
| H-HW-0.417000 | 0 | 3.29341 | -2.42737 | 4.16018 | H |
| O-OW--0.834000 | 0 | 1.69999 | -12.48685 | -5.59016 | L |
| H-HW-0.417000 | 0 | 2.06087 | -12.08434 | -6.39123 | L |
| H-HW-0.417000 | 0 | 0.89036 | -11.94158 | -5.41837 | L |
| O-OW--0.834000 | 0 | 6.86664 | -7.96803 | -7.60044 | L |
| H-HW-0.417000 | 0 | 6.46791 | -7.14686 | -7.27029 | L |
| H-HW-0.417000 | 0 | 6.15571 | -8.60686 | -7.42938 | L |
| O-OW--0.834000 | 0 | 2.04276 | -7.43602 | -1.63413 | L |
| H-HW-0.417000 | 0 | 1.32947 | -6.77018 | -1.5535 | L |

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H-HW-0.417000        0     2.40817  -7.2209   -2.51257  L
O-OW--0.834000       0     1.91125  -10.78827  -3.3511   L
H-HW-0.417000        0     2.05632  -11.68938  -3.68022  L
H-HW-0.417000        0     1.0929   -10.53824  -3.85901  L
O-OW--0.834000       0    -7.78199  -5.60973   0.15355  L
H-HW-0.417000        0    -8.26032  -4.95548   0.68902  L
H-HW-0.417000        0    -8.24969  -6.43513   0.35415  L
O-OW--0.834000       0     2.53817  -10.80062  -7.77638  L
H-HW-0.417000        0     2.70263  -11.21736  -8.62702  L
H-HW-0.417000        0     1.55859  -10.72491  -7.76161  L
O-OW--0.834000       0    -3.29997  -3.01461  -13.34003  L
H-HW-0.417000        0    -2.94411  -3.90869  -13.34395  L
H-HW-0.417000        0    -3.286    -2.79859  -12.38296  L
O-OW--0.834000       0     9.40975  -8.25673  -8.43165  L
H-HW-0.417000        0     9.21087  -8.62313  -9.29642  L
H-HW-0.417000        0     8.51177  -8.12547  -8.05178  L
O-OW--0.834000       0     1.96952  -6.79503   1.34286  H
H-HW-0.417000        0     1.46611  -6.59597   2.16859  H
H-HW-0.417000        0     2.04738  -5.92074   0.92643  H
O-OW--0.834000       0    -0.30713  -8.38167   0.17531  L
H-HW-0.417000        0     0.55972  -7.95168   0.1203   L
H-HW-0.417000        0    -0.44249  -8.71597  -0.72442  L
O-OW--0.834000       0     4.27648  -3.88838   3.86413  L
H-HW-0.417000        0     4.21373  -4.00685   2.89564  L
H-HW-0.417000        0     4.05252  -4.7698    4.20953  L
O-OW--0.834000       0     1.20657  -5.58696   3.66953  H
H-HW-0.417000        0     0.98903  -4.69022   3.31964  H
H-HW-0.417000        0     0.36917  -5.83691   4.14032  H
O-OW--0.834000       0    -0.7287   -9.32821  -2.5524   L
H-HW-0.417000        0    -0.30655  -8.49503  -2.82424  L
H-HW-0.417000        0    -0.75813  -9.78608  -3.43852  L
C-CW--0.220700       0     7.96784  -10.31675   10.71961  L
H-H4-0.186200        0     9.00256  -10.25018   10.4096  L
C-CT--0.149000       0     12.54685  -3.42169   12.99843  L
H-H1-0.097600        0     12.51948  -2.57259   13.68349  L
H-H1-0.097600        0     12.06393  -4.28058   13.46497  L
H-H1-0.097600        0     13.59045  -3.66458   12.78846  L
H-HC                 0    -6.87952  -10.34428  -7.49418  L
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**TS1**

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N-N--0.347900        0    -7.45077   15.28006   3.77968  L
 C-CT--0.263700       -1   -7.37751   13.91778   4.32822  L
 C-C-0.734100          0    -6.56356   13.04322   3.3775   L
 O-O--0.589400         0    -6.93621   12.9157   2.21766  L
 C-CT--0.000700        0    -8.79936   13.33001   4.49022  L
 C-CT-0.039000         0    -9.58115   13.91296   5.67898  L
 C-CT-0.048600         0    -11.0086   13.34011   5.79982  L
 N-N2--0.529502        0    -11.06576   11.93717   6.27455  L
 C-CA-0.807600         0    -10.98398   11.49978   7.52023  L
 N-N2--0.862702        0    -10.68625   12.27911   8.52252  L
 N-N2--0.862702        0    -11.21478   10.24891   7.78234  L
 H-H-0.274700          0    -7.23614   15.40269   2.78976  L
 H-H-0.274700          0    -7.49212   16.09578   4.37852  L
 H-H1-0.156001         0    -6.87406   13.93139   5.29527  L
 H-HC-0.032700         0    -8.72764   12.25034   4.61813  L
 H-HC-0.032700         0    -9.36316   13.51218   3.57619  L
 H-HC-0.028500         0    -9.66325   14.99188   5.5414   L
 H-HC-0.028500         0    -9.03239   13.73061   6.6033   L
 H-H1-0.068701         0    -11.49938   13.40896   4.8267   L
 H-H1-0.068701         0    -11.57715   13.97023   6.4873   L
 H-H-0.345600          0    -11.35415   11.21808   5.61945  L
 H-H-0.447800          0    -10.65127   11.91503   9.45705  L
 H-H-0.447800          0    -10.5487   13.25705   8.35084  L
 H-H-0.447800          0    -11.18385   9.87926   8.71279  L
 H-H-0.447800          0    -11.52928   9.66226   7.01077  L
 N-N--0.415700         0    -5.49057   12.43944   3.88394  L
 C-CT--0.087500       -1   -4.51521   11.64879   3.11896  L
 C-C-0.597300          0    -4.39016   10.24773   3.69794  L
 O-O--0.567900         0    -4.35879   10.10095   4.92184  L
 C-CT-0.298500         0    -3.17795   12.40604   3.00894  L
 C-CT--0.319200        0    -2.51892   12.65683   4.36713  L
 C-CT--0.319200        0    -2.20454   11.68809   2.07259  L
 H-H-0.271900          0    -5.28523   12.56229   4.86213  L
 H-H1-0.096900         0    -4.89549   11.52975   2.10615  L
 H-HC--0.029700        0    -3.3862    13.38203   2.56943  L
 H-HC-0.079100         0    -3.18242   13.21623   5.02328  L
 H-HC-0.079100         0    -1.61151   13.24557   4.22387  L
 H-HC-0.079100         0    -2.24781   11.71334   4.83907  L
 H-HC-0.079100         0    -1.28324   12.26646   1.9913   L
 H-HC-0.079100         0    -2.64762   11.60152   1.08114  L
 H-HC-0.079100         0    -1.96488   10.69624   2.44858  L
 N-N--0.347900         0    -4.40263   9.21682   2.838    L
 C-CT--0.263700       -1   -4.59158   7.82757   3.28868  L
 C-C-0.734100          0    -3.43564   6.86428   3.09216  L
 O-O--0.589400         0    -2.52377   7.10874   2.3134   L
 C-CT--0.000700        0    -5.96234   7.24017   2.88252  L
 C-CT-0.039000         0    -6.01964   6.15626   1.78816  L    H-H1
48    0.        0.
 C-CT-0.048600         0    -5.39472   6.55931   0.45018  H
 N-N2--0.529500        0    -5.67589   5.59127  -0.59933  H
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 C-CA-0.807600         0    -4.99761   4.44062  -0.8146   H
 N-N2--0.862700        0    -3.71357   4.31346  -0.46345  H
 N-N2--0.862700        0    -5.63591   3.41701  -1.36103  H
 H-H-0.274700          0    -4.39822   9.43279   1.8484   L
 H-H1-0.156000         0    -4.6488    7.87438   4.3766   L
 H-HC-0.032700         0    -6.62463   8.05262   2.6134   L
 H-HC-0.032700         0    -6.39792   6.78659   3.77455  L
 H-HC-0.028500         0    -7.07115   5.92606   1.6178   L
 H-HC-0.028500         0    -5.54612   5.24038   2.14169  L
 H-H1-0.068700         0    -4.3191    6.67845   0.55956  H
 H-H1-0.068700         0    -5.80624   7.51728   0.14905  H
 H-H-0.345600          0    -6.6626    5.48228  -0.86258  H
 H-H-0.447800          0    -3.23385   3.44987  -0.79806  H
 H-H-0.447800          0    -3.1662    5.17643  -0.42257  H
 H-H-0.447800          0    -5.14434   2.58746  -1.80183  H
 H-H-0.447800          0    -6.64097   3.59722  -1.51679  H
 N-N--0.415700         0    -3.51012   5.74868   3.80544  L
 C-CT--0.002400       -1    -2.5939    4.62743   3.73271  L
 C-C-0.597300          0    -3.30704   3.30816   4.04881  L
 O-O--0.567900         0    -4.10207   3.23812   4.98596  L
 C-CT--0.034300        0    -1.43939   4.91287   4.7108   L
 C-CA-0.011800         0    -0.47196   3.77222   4.97205  L
 C-CA--0.125600        0     0.29261   3.21437   3.92937  L
 C-CA--0.125600        0    -0.32447   3.27733   6.28069  L
 C-CA--0.170400        0     1.19202   2.16515   4.20108  L
 C-CA--0.170400        0     0.56334   2.22116   6.54793  L
 C-CA--0.107200        0     1.32492   1.66549   5.50653  L
 H-H-0.271900          0    -4.22513   5.7012    4.52362  L
 H-H1-0.097800         0    -2.18675   4.56189   2.72221  L
 H-HC-0.029500         0    -1.87163   5.22141   5.66469  L
 H-HC-0.029500         0    -0.8657    5.75945   4.33071  L
 H-HA-0.133000         0     0.19313   3.5925    2.9228   L
 H-HA-0.133000         0    -0.91015   3.70106   7.08073  L
 H-HA-0.143000         0     1.79803   1.72916   3.41948  L
 H-HA-0.143000         0     0.64281   1.82298   7.547    L
 H-HA-0.129700         0     2.00826   0.84785   5.69694  L
 N-N--0.415700         0    -3.02702   2.27299   3.25296  L
 C-CT-0.033700        -1    -3.81061   1.03915   3.20394  L
 C-C-0.597300          0    -2.94314  -0.23328   3.33486  L
 O-O--0.567900         0    -2.811    -0.99296   2.3808   L
 C-CT--0.182500        0    -4.6527    1.12052   1.92468  L
 H-H-0.271900          0    -2.36493   2.41457   2.5068   L
 H-H1-0.082300         0    -4.51439   1.02072   4.03389  L
 H-HC-0.060300         0    -4.00898   1.26339   1.05715  L
 H-HC-0.060300         0    -5.34865   1.95819   1.98984  L
 H-HC-0.060300         0    -5.22399   0.20638   1.80341  L
 N-N--0.254800         0    -2.32775  -0.52183   4.4926   L
 C-CT--0.026600        0    -1.58769  -1.76519   4.70207  L    H-H2
98    0.        0.
 C-C-0.589600          0    -2.49939  -3.01354   4.57622  H
 O-O--0.574800         0    -3.48173  -3.21435   5.27024  H
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 C-CT--0.007000       0    -0.95059  -1.63986   6.09195  L
 C-CT-0.018900        0    -1.80759  -0.58462   6.78929  L
 C-CT-0.019200        0    -2.18925   0.34414   5.64512  L
 H-H1-0.064100        0    -0.79038  -1.82837   3.96394  L
 H-HC-0.025300        0     0.06948  -1.26686   5.99162  L
 H-HC-0.025300        0    -0.95606  -2.58572   6.63528  L
 H-HC-0.021300        0    -1.26437  -0.06064   7.5751   L
 H-HC-0.021300        0    -2.70819  -1.05302   7.18095  L
 H-H1-0.039100        0    -3.09126   0.90281   5.87958  L
 H-H1-0.039100        0    -1.3814    1.03696   5.4409   L
 N-N--0.415700        0    -2.09663  -3.88805   3.60625  H
 C-CT--0.024900       0    -2.52854  -5.27161   3.66132  H
 C-C-0.597300         0    -1.95688  -5.96261   4.90922  L    H-H1
111   0.        0.
 O-O--0.567900        0    -0.76111  -5.82934   5.17443  L
 C-CT-0.211700        0    -2.07918  -6.08305   2.45834  H
 O-OH--0.654600       0    -2.84756  -5.85875   1.30631  H
 H-H-0.271900         0    -1.19593  -3.71669   3.17024  H
 H-H1-0.084300        0    -3.61645  -5.28388   3.69851  H
 H-H1-0.035200        0    -2.19081  -7.14034   2.72076  H
 H-H1-0.035200        0    -1.00637  -5.89959   2.27043  H
 H-HO-0.427500        0    -2.36615  -5.26722   0.71639  H
 N-N--0.254800        0    -2.7729   -6.71531   5.66603  L
 C-CT--0.026600       0    -2.32559  -7.55317   6.76283  L
 C-C-0.589600         0    -1.79494  -8.88203   6.19895  L
 O-O--0.574800        0    -2.39193  -9.93603   6.40388  L
 C-CT--0.007000       0    -3.58062  -7.72254   7.62615  L
 C-CT-0.018900        0    -4.70649  -7.78162   6.59988  L
 C-CT-0.019200        0    -4.20333  -6.87673   5.48067  L
 H-H1-0.064100        0    -1.54561  -7.05291   7.33552  L
 H-HC-0.025300        0    -3.71013  -6.83349   8.23876  L
 H-HC-0.025300        0    -3.55656  -8.61186   8.25624  L
 H-HC-0.021300        0    -5.63421  -7.40182   7.01938  L
 H-HC-0.021300        0    -4.83325  -8.79958   6.22889  L
 H-H1-0.039100        0    -4.4026   -7.34152   4.51515  L
 H-H1-0.039100        0    -4.68902  -5.90522   5.55447  L
 N-N--0.415700        0    -0.67123  -8.83956   5.48155  L
 C-CT--0.038900      -1    -0.1511   -9.97624   4.70519  L
 C-C-0.597300         0     1.35425  -10.21266   4.93145  L
 O-O--0.567900        0     2.12408  -10.44761   3.99684  L
 C-CT-0.365400        0    -0.47968  -9.84323   3.19842  L
 O-OH--0.676100       0    -0.06455  -8.59709   2.66575  L
 C-CT--0.243800       0    -1.97574  -9.99547   2.92009  L
 H-H-0.271900         0    -0.19519  -7.94959   5.35979  L
 H-H1-0.100700        0    -0.63205  -10.89536   5.04303  L
 H-H1-0.004300        0     0.02868  -10.63935   2.65338  L
 H-HC-0.064200        0    -2.54575  -9.2258    3.43738  L
 H-HC-0.064200        0    -2.3114   -10.97356   3.26555  L
 H-HC-0.064200        0    -2.16084  -9.91973   1.84834  L
 H-HO-0.410200        0    -0.31084  -8.60064   1.71494  L
 N-N--0.415700        0     1.79775  -10.16876   6.19189  L
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C-CT--0.025200       -1    3.19743  -10.31337   6.6115   L
C-C-0.597300         0     3.73753  -9.11748   7.42897  L
O-O--0.567900        0     3.01332  -8.16406   7.72551  L
H-H-0.271900         0     1.11031  -9.99144   6.90941  L
H-H1-0.069800        0     3.83571  -10.43419   5.738    L
H-H1-0.069800        0     3.29188  -11.21612   7.21161  L
N-N--0.415700        0     5.02403  -9.14758   7.79763  L
C-CT--0.058100       -1    5.71317  -8.06747   8.53864  L
C-C-0.597300         0     5.87097  -6.78839   7.69585  L
O-O--0.567900        0     6.0683   -6.84813   6.48268  L
C-CT--0.007400       0     7.08819  -8.5642    9.01243  L
C-CC-0.186800        0     7.0357   -9.68709   10.02195  L
N-NB--0.543200       0     5.90255  -10.10765   10.72076  L
C-CR-0.163500        0     6.31594  -11.0876   11.53798  L
N-NA--0.279500       0     7.63427  -11.30456   11.3815  L
H-H-0.271900         0     5.56087  -9.96677   7.56239  L
H-H1-0.136000        0     5.1156   -7.82085   9.41736  L
H-HC-0.036700        0     7.62124  -7.73226   9.47435  L
H-HC-0.036700        0     7.66732  -8.89307   8.14816  L
H-H-0.333900         0     8.17776  -11.98548   11.89675  L
H-H5-0.143500        0     5.67786  -11.62067   12.23169  L
N-N--0.415700        0     5.8186   -5.62694   8.35691  L
C-CT--0.051800       0     6.01502  -4.29937   7.76064  L
C-C-0.597300         0     7.44513  -4.11487   7.22626  L
O-O--0.567900        0     8.4048   -4.1747    7.99914  L
C-CT--0.110200       0     5.72231  -3.24198   8.84269  L
C-CT-0.353100        0     5.93495  -1.78121   8.39652  L
C-CT--0.412100       0     4.90385  -1.29878   7.37605  L
C-CT--0.412100       0     5.86168  -0.8754    9.6229   L
H-H-0.271900         0     5.68429  -5.67454   9.35314  L
H-H1-0.092200        0     5.31076  -4.17788   6.93485  L
H-HC-0.045700        0     6.38542  -3.43662   9.68773  L
H-HC-0.045700        0     4.70216  -3.36246   9.19463  L
H-HC--0.036100       0     6.9235   -1.66926   7.96014  L
H-HC-0.100000        0     3.90722  -1.29585   7.80737  L
H-HC-0.100000        0     4.91806  -1.93457   6.49044  L
H-HC-0.100000        0     5.14227  -0.28353   7.07033  L
H-HC-0.100000        0     4.88591  -0.97243   10.097   L
H-HC-0.100000        0     6.02639   0.15885   9.32664  L
H-HC-0.100000        0     6.63602  -1.15865   10.33606  L
N-N--0.415700        0     7.58065  -3.79163   5.93839  L
C-CT--0.058100       -1    8.85466  -3.414     5.31088  L
C-C-0.597300         0     8.97551  -1.90534   5.08991  L
O-O--0.567900        0     8.00017  -1.14993   5.13826  L
C-CT--0.007400       0     9.0529   -4.20526   4.01083  L
C-CC-0.186800        0     8.10345  -3.82215   2.90817  L
N-NB--0.543200       0     8.31723  -2.79763   1.98616  L
C-CW--0.220700       0     6.92122  -4.44232   2.6346   L
C-CR-0.163500        0     7.27516  -2.8613    1.13933  L
N-NA--0.279500       0     6.40816  -3.81529   1.52119  L
H-H-0.271900         0     6.74175  -3.73567   5.37637  L
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H-H1-0.136000        0     9.67014  -3.69343   5.97631  L
H-HC-0.036700        0     8.94474  -5.27052   4.22013  L
H-HC-0.036700        0     10.06894  -4.04762   3.64808  L
H-H4-0.186200        0     6.48498  -5.27153   3.17453  L
H-H-0.333900         0     5.52053  -4.03073   1.06422  L
H-H5-0.143500        0     7.14696  -2.22973   0.27212  L
N-N--0.415700        0     10.21197  -1.46867   4.86369  L
C-CT--0.087500       -1    10.60062  -0.05999   4.71117  L
C-C-0.597300         0     9.85608   0.69161   3.60789  L
O-O--0.567900        0     9.5404    1.85904   3.80592  L
C-CT-0.298500        0     12.12585   0.07894   4.54452  L
C-CT--0.319200       0     12.84338  -0.30734   5.84388  L
C-CT--0.319200       0     12.68749  -0.77152   3.39939  L
H-H-0.271900         0     10.9466  -2.16896   4.87168  L
H-H1-0.096900        0     10.33711   0.45143   5.63614  L
H-HC--0.029700       0     12.35397   1.12263   4.33558  L
H-HC-0.079100        0     12.6819  -1.36037   6.07839  L
H-HC-0.079100        0     12.47753   0.30331   6.6688   L
H-HC-0.079100        0     13.91437  -0.13607   5.73618  L
H-HC-0.079100        0     12.49772  -1.83068   3.57193  L
H-HC-0.079100        0     13.76436  -0.63266   3.33478  L
H-HC-0.079100        0     12.24871  -0.46584   2.45142  L
N-N--0.415700        0     9.53849   0.06406   2.47171  L
C-CT--0.025200       -1    8.76369   0.6962    1.39721  L
C-C-0.597300         0     7.3258    1.0175    1.82557  L
O-O--0.567900        0     6.86094   2.13688   1.61386  L
H-H-0.271900         0     9.73763  -0.92676   2.40126  L
H-H1-0.069800        0     8.72719   0.03094   0.53416  L
H-H1-0.069800        0     9.24548   1.62476   1.1015   L
N-N--0.415700        0     6.63262   0.06691   2.46193  L
C-CT--0.025200       0     5.3109    0.27607   3.07185  L
C-C-0.597300         0     5.32766   1.37324   4.14519  L
O-O--0.567900        0     4.55282   2.3287    4.09064  L
H-H-0.271900         0     7.08833  -0.82897   2.59754  L
H-H1-0.069800        0     4.96948  -0.6529    3.52958  L
H-H1-0.069800        0     4.59585   0.55832   2.29814  L
N-N--0.415700        0     6.24789   1.27174   5.10966  L
C-CT-0.033700        -1    6.46078   2.27519   6.16023  L
C-C-0.597300         0     6.77538   3.66972   5.59907  L
O-O--0.567900        0     6.29804   4.66991   6.12897  L
C-CT--0.182500       0     7.57449   1.77818   7.07483  L
H-H-0.271900         0     6.84735   0.45123   5.09058  L
H-H1-0.082300        0     5.54008   2.35574   6.73677  L
H-HC-0.060300        0     7.31455   0.77978   7.41378  L
H-HC-0.060300        0     7.67641   2.44305   7.93328  L
H-HC-0.060300        0     8.51986   1.73895   6.53256  L
N-N--0.347900        0     7.5621    3.75178   4.52162  L
C-CT--0.263700       -1    7.81693   4.98458   3.77245  L
C-C-0.734100         0     6.5361    5.63088   3.23233  L
O-O--0.589400        0     6.45152   6.84943   3.29889  L
C-CT--0.000700       0     8.93406   4.74179   2.74229  L
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C-CT-0.039000        0     9.22641   5.89079   1.75987  L
C-CT-0.048600        0     8.28584   5.78064   0.55825  L
N-N2--0.529500       0     8.75666   6.51092  -0.62074  L
C-CA-0.807600        0     8.63223   6.10444  -1.86755  L
N-N2--0.862700       0     7.92907   5.0696   -2.21385  L
N-N2--0.862700       0     9.23931   6.73831  -2.81826  L
H-H-0.274700         0     7.98883   2.89204   4.18776  L
H-H1-0.156000        0     8.20882   5.71399   4.47988  L
H-HC-0.032700        0     8.72423   3.833     2.18073  L
H-HC-0.032700        0     9.84778   4.55019   3.30281  L
H-HC-0.028500        0     10.25233   5.77932   1.40548  L
H-HC-0.028500        0     9.12576   6.86181   2.24661  L
H-H1-0.068700        0     7.28483   6.12419   0.81763  L
H-H1-0.068700        0     8.24931   4.7259    0.2972   L
H-H-0.345600         0     9.29723   7.3628   -0.50425  L
H-H-0.447800         0     7.92005   4.81317  -3.19309  L
H-H-0.447800         0     7.31945   4.61456  -1.53711  L
H-H-0.447800         0     9.23413   6.31755  -3.7375   L
H-H-0.447800         0     9.78902   7.5467   -2.55188  L
N-N--0.415700        0     5.53393   4.87994   2.76258  L
C-CT--0.038900      -1     4.19863   5.43684   2.43435  L
C-C-0.597300         0     3.56569   6.10713   3.65258  L
O-O--0.567900        0     3.11508   7.24215   3.54957  L
C-CT-0.365400        0     3.22646   4.36757   1.89651  L
O-OH--0.676100       0     3.82898   3.53987   0.93053  L
C-CT--0.243800       0     2.0135    4.99297   1.21027  L
H-H-0.271900         0     5.66821   3.87809   2.69865  L
H-H1-0.100700        0     4.32585   6.19819   1.664    L
H-H1-0.004300        0     2.88934   3.74126   2.71949  L
H-HC-0.064200        0     1.44602   5.5903    1.92321  L
H-HC-0.064200        0     1.36812   4.20956   0.81433  L
H-HC-0.064200        0     2.34088   5.63254   0.38947  L
H-HO-0.410200        0     3.3224    2.71486   0.9013   L
N-N--0.415700        0     3.54353   5.43253   4.8102   L
C-CT-0.033700       -1     3.0793    6.01994   6.07218  L
C-C-0.597300         0     3.82878   7.31192   6.41972  L
O-O--0.567900        0     3.18909   8.32746   6.64768  L
C-CT--0.182500       0     3.1321    4.97749   7.18739  L
H-H-0.271900         0     3.92869   4.49661   4.81858  L
H-H1-0.082300        0     2.0339    6.29691   5.93543  L
H-HC-0.060300        0     2.58062   4.09007   6.88177  L
H-HC-0.060300        0     2.67871   5.39312   8.08762  L
H-HC-0.060300        0     4.16152   4.70741   7.40347  L
N-N--0.415700        0     5.16406   7.28826   6.42311  L
C-CT--0.051800      -1     6.0289    8.45131   6.64733  L
C-C-0.597300         0     5.72171   9.61742   5.71249  L
O-O--0.567900        0     5.54008   10.73831   6.17294  L
C-CT--0.110200       0     7.49714   7.9921    6.53414  L
C-CT-0.353100        0     8.54579   9.09261   6.78856  L
C-CT--0.412100       0     8.54859   9.55747   8.24461  L
C-CT--0.412100       0     9.94005   8.55315   6.45615  L
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H-H-0.271900          0      5.59812   6.3911    6.23698  L
H-H1-0.092200         0      5.85021   8.80612   7.66331  L
H-HC-0.045700         0      7.65316   7.60811   5.52808  L
H-HC-0.045700         0      7.66698   7.17316   7.23485  L
H-HC--0.036100        0      8.35404   9.94667   6.1402   L
H-HC-0.100000         0      9.32291   10.31038   8.39153  L
H-HC-0.100000         0      8.72909   8.71699   8.91418  L
H-HC-0.100000         0      7.58985   10.01262   8.49065  L
H-HC-0.100000         0      10.16637   7.69507   7.089    L
H-HC-0.100000         0      10.67877   9.33614   6.62644  L
H-HC-0.100000         0      9.97359   8.25821   5.40739  L
N-N--0.415700         0      5.69487   9.35145   4.41024  L
C-CT--0.002400        -1     5.41067   10.33717   3.37874  L
C-C-0.597300          0      4.02556   10.96755   3.55151  L
O-O--0.567900         0      3.89058   12.18645   3.57785  L
C-CT--0.034300        0      5.58393   9.6811    1.99609  L
C-CA-0.011800         0      5.65      10.64732   0.82601  L
C-CA--0.125600        0      6.89751   10.99996   0.27364  L
C-CA--0.125600        0      4.4712    11.17596   0.26605  L
C-CA--0.170400        0      6.96529   11.87718  -0.82386  L
C-CA--0.170400        0      4.53769   12.05434  -0.83019  L
C-CA--0.107200        0      5.78492   12.4068  -1.37442  L
H-H-0.271900          0      5.86131   8.39646   4.11573  L
H-H1-0.097800         0      6.13838   11.14541   3.46461  L
H-HC-0.029500         0      4.77204   8.97225   1.8248   L
H-HC-0.029500         0      6.51274   9.11012   1.99959  L
H-HA-0.133000         0      7.81069   10.60125   0.69021  L
H-HA-0.133000         0      3.50781   10.91457   0.6774   L
H-HA-0.143000         0      7.92579   12.15091  -1.23844  L
H-HA-0.143000         0      3.62753   12.45921  -1.25148  L
H-HA-0.129700         0      5.834     13.08782  -2.21228  L
N-N--0.415700         0      2.99655   10.13115   3.68383  L
C-CT-0.014300         -1     1.61135   10.56375   3.82532  L
C-C-0.597300          0      1.29663   11.15258   5.23107  L
O-O--0.567900         0      0.29244   11.84224   5.3807   L
C-CT--0.204100        0      0.67994   9.39099   3.45319  L
C-C-0.713000          0      0.76681   8.97659   1.9866   L
O-O--0.593100         0      1.51704   9.49503   1.18065  L
N-N--0.919100         0     -0.02167   8.02727   1.55067  L
H-H-0.271900          0      3.1869    9.13744   3.6259   L
H-H1-0.104800         0      1.43276   11.37465   3.11567  L
H-HC-0.079700         0     -0.34695   9.67837   3.66533  L
H-HC-0.079700         0      0.92584   8.53018   4.06982  L
H-H-0.419600          0      0.09822   7.81964   0.57872  L
H-H-0.419600          0     -0.79451   7.63898   2.07747  L
N-N--0.415700         0      2.10242   10.87764   6.26641  L
C-CT--0.027500        -1     2.11737   11.56369   7.57575  L
C-C-0.597300          0      2.76401   12.95941   7.45954  L
N-N--0.415700         0      3.96379   13.04251   6.86455  L
C-CT--0.149000        -1     4.74783   14.25852   6.64905  L
O-O--0.567900         0      2.17338   13.94018   7.90852  L
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C-CT--0.005000       0     2.84639   10.68468   8.60116  L
C-C*--0.141500       0     3.1655    11.32713   9.91479  L
C-CW--0.163800       0     2.30355   11.50733   10.94092  L
C-CB-0.124300        0     4.43853   11.89755   10.34867  L
N-NA--0.341800       0     2.95825   12.13956   11.98313  L
C-CN-0.138000        0     4.27768   12.39664   11.67425  L
C-CA--0.238700       0     5.70953   12.05221   9.75242  L
C-CA--0.260100       0     5.32606   13.00439   12.38133  L
C-CA--0.197200       0     6.77034   12.66127   10.4511  L
C-CA--0.113400       0     6.58183   13.13418   11.76271  L
H-H-0.271900         0     2.83113   10.19351   6.10491  L
H-H-0.271900         0     4.35761   12.17489   6.51871  L
H-H1-0.112300        0     1.09422   11.71868   7.91556  L
H-HC-0.033900        0     3.79139   10.35666   8.1704   L
H-HC-0.033900        0     2.24364   9.79449   8.78604  L
H-H4-0.206200        0     1.26315   11.2096   10.92831  L
H-H-0.341200         0     2.51807   12.41587   12.84829  L
H-HA-0.170000        0     5.852     11.71438   8.73635  L
H-HA-0.157200        0     5.16666   13.37822   13.38132  L
H-HA-0.144700        0     7.73223   12.78105   9.97232  L
H-HA-0.141700        0     7.39853   13.61064   12.2882  L
H-H1-0.097600        0     5.22114   14.56028   7.5847   L
H-H1-0.097600        0     4.09218   15.06135   6.30677  L
H-H1-0.097600        0     5.5118    14.07417   5.89275  L
N-N--0.415700        0    -3.76183   12.29362   8.44293  L
C-CT--0.002400      -1    -3.39419   10.92388   8.08653  L
C-C-0.597300         0    -4.51017   9.93287   8.44168  L
O-O--0.567900        0    -5.18715   10.09536   9.45634  L
C-CT--0.034300       0    -2.0774    10.58526   8.79835  L
C-CA-0.011800        0    -1.5094    9.21829   8.47243  L
C-CA--0.125600       0    -0.9612    8.97056   7.20053  L
C-CA--0.125600       0    -1.49762   8.20328   9.44818  L
C-CA--0.170400       0    -0.39281   7.71829   6.91071  L
C-CA--0.170400       0    -0.9214    6.95365   9.15982  L
C-CA--0.107200       0    -0.36584   6.71238   7.89147  L
H-H-0.271900         0    -4.44348   12.39063   9.1863   L
H-H-0.271900         0    -3.08866   13.03098   8.27429  L
H-H1-0.097800        0    -3.22071   10.88016   7.01157  L
H-HC-0.029500        0    -2.22946   10.66191   9.87639  L
H-HC-0.029500        0    -1.32968   11.3307   8.52133  L
H-HA-0.133000        0    -0.95541   9.75027   6.45186  L
H-HA-0.133000        0    -1.91312   8.38726   10.42894  L
H-HA-0.143000        0     0.04418   7.53913   5.94072  L
H-HA-0.143000        0    -0.89373   6.18838   9.92152  L
H-HA-0.129700        0     0.095     5.76167   7.67179  L
N-N--0.415700        0    -4.72574   8.93218   7.58719  L
C-CT--0.059700      -1    -5.73207   7.8777    7.74311  L
C-C-0.597300         0    -5.07233   6.52407   7.47223  L
O-O--0.567900        0    -4.45407   6.35908   6.42073  L
C-CT-0.130300        0    -6.9542    8.11092   6.81738  L
C-CT--0.043000       0    -7.76029   9.38554   7.16971  L
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C-CT--0.320400       0    -7.91761   6.91096   6.91285  L
C-CT--0.066000       0    -7.27372   10.67169   6.49108  L
H-H-0.271900         0    -4.16304   8.9152    6.74442  L
H-H1-0.086900        0    -6.08541   7.87231   8.77497  L
H-HC-0.018700        0    -6.61561   8.18277   5.78319  L
H-HC-0.023600        0    -7.77161   9.52673   8.25128  L
H-HC-0.023600        0    -8.79211   9.25099   6.84648  L
H-HC-0.088200        0    -8.23544   6.75345   7.94433  L
H-HC-0.088200        0    -7.44756   6.0002    6.53908  L
H-HC-0.088200        0    -8.79838   7.07847   6.2959   L
H-HC-0.018600        0    -6.27981   10.95003   6.82538  L
H-HC-0.018600        0    -7.95401   11.48235   6.74591  L
H-HC-0.018600        0    -7.25937   10.53687   5.41055  L
N-N--0.415700        -1   -5.22604   5.55729   8.38859  L
C-CT--0.051800       0    -4.63117   4.22663   8.25776  L
C-C-0.597300         0    -5.74201   3.18225   8.26872  L
O-O--0.567900        0    -6.45884   3.05083   9.26004  L
C-CT--0.110200       0    -3.57542   4.01933   9.36194  L
C-CT-0.353100        0    -2.74631   2.72294   9.21714  L
C-CT--0.412100       0    -1.39705   2.8848    9.9248   L
C-CT--0.412100       0    -3.41512   1.48833   9.82701  L
H-H-0.271900         0    -5.78959   5.73704   9.20572  L
H-H1-0.092200        0    -4.11418   4.15526   7.30071  L
H-HC-0.045700        0    -4.05309   4.04239   10.34272  L
H-HC-0.045700        0    -2.89403   4.86791   9.30681  L
H-HC--0.036100       0    -2.55609   2.53001   8.16202  L
H-HC-0.100000        0    -0.80392   1.97918   9.80209  L
H-HC-0.100000        0    -1.55629   3.07045   10.98773  L
H-HC-0.100000        0    -0.84832   3.72067   9.49353  L
H-HC-0.100000        0    -3.68222   1.68022   10.86657  L
H-HC-0.100000        0    -2.73604   0.6381    9.78261  L
H-HC-0.100000        0    -4.31407   1.22539   9.27485  L
N-N--0.347900        0    -5.8573    2.43213   7.17197  L
C-CT--0.263700       -1   -6.78522   1.31182   7.03051  L
C-C-0.734100         0    -6.03123  -0.0139    6.894    L
O-O--0.589400        0    -5.18687  -0.15177   6.01836  L
C-CT--0.000700       0    -7.69122   1.52374   5.8129   L
C-CT-0.039000        0    -8.57593   0.28222   5.61003  L
C-CT-0.048600        0    -9.68418   0.52077   4.60771  L
N-N2--0.529500       0    -9.1688    0.7159    3.24552  L
C-CA-0.807600        0    -9.15427   1.81874   2.52952  L
N-N2--0.862700       0    -9.76304   2.91963   2.85234  L
N-N2--0.862700       0    -8.49744   1.8098    1.41726  L
H-H-0.274700         0    -5.23754   2.63939   6.39195  L
H-H1-0.156000        0    -7.419     1.24492   7.91731  L
H-HC-0.032700        0    -7.08465   1.68794   4.91991  L
H-HC-0.032700        0    -8.31328   2.40167   5.9807   L
H-HC-0.028500        0    -9.0362    0.00396   6.55932  L
H-HC-0.028500        0    -7.97155  -0.54563   5.24832  L
H-H1-0.068700        0    -10.22848   1.39298   4.95143  L
H-H1-0.068700        0    -10.34846  -0.34312   4.6198   L
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 H-H-0.345600          0    -8.73038  -0.0656    2.76647  L
 H-H-0.447800          0    -9.71455   3.66261   2.15926  L
 H-H-0.447800          0    -10.54278   2.86754   3.51463  L
 H-H-0.447800          0    -8.51694   2.66712   0.8647   L
 H-H-0.447800          0    -8.11834   0.92087   1.09763  L
 N-N--0.415700         0    -6.38086  -1.01524   7.69663  L
 C-CT--0.059700       -1    -5.97357  -2.4084    7.45136  L
 C-C-0.597300          0    -6.88887  -3.02156   6.38246  L
 O-O--0.567900         0    -8.09755  -2.80694   6.40967  L
 C-CT-0.130300         0    -6.11655  -3.22252   8.76047  L
 C-CT--0.043000        0    -5.3754   -2.61214   9.974    L
 C-CT--0.320400        0    -5.67499  -4.68117   8.55433  L
 C-CT--0.066000        0    -3.89446  -2.28357   9.74779  L
 H-H-0.271900          0    -7.15214  -0.85322   8.33251  L
 H-H1-0.086900         0    -4.94019  -2.44084   7.10912  L
 H-HC-0.018700         0    -7.17551  -3.24626   9.02658  L
 H-HC-0.023600         0    -5.452    -3.30145   10.81581  L
 H-HC-0.023600         0    -5.88324  -1.69389   10.27233  L
 H-HC-0.088200         0    -6.34918  -5.18397   7.86049  L
 H-HC-0.088200         0    -5.72455  -5.22057   9.49874  L
 H-HC-0.088200         0    -4.66074  -4.71242   8.15709  L
 H-HC-0.018600         0    -3.44266  -1.98474   10.69386  L
 H-HC-0.018600         0    -3.8118   -1.45497   9.0493   L
 H-HC-0.018600         0    -3.35904  -3.14623   9.35428  L
 N-N--0.516300         0    -6.35306  -3.82576   5.4687   L
 C-CT-0.039700        -1    -7.13637  -4.38457   4.35963  L
 C-C-0.536600          0    -7.21286  -5.91798   4.33554  L
 O-O--0.581900         0    -6.502    -6.57332   3.5762   L
 C-CT-0.056000         0    -6.59911  -3.80899   3.02028  L    H-HC
485   0.        0.
 C-CT-0.013600         0    -6.76305  -2.28055   2.90306  H
 C-C-0.805400          0    -7.01753  -1.68632   1.51601  H
 O-O2--0.818800        0    -6.18168  -1.90427   0.51573  H
 O-O2--0.818800        0    -7.95862  -0.93047   1.34934  H
 H-H-0.293600          0    -5.33969  -3.86421   5.43407  L
 H-H1-0.110500         0    -8.17221  -4.05323   4.42821  L
 H-HC--0.017300        0    -7.14878  -4.27243   2.20842  L
 H-HC--0.017300        0    -5.54582  -4.06543   2.89733  L
 H-HC--0.042500        0    -5.87539  -1.81585   3.34438  H
 H-HC--0.042500        0    -7.63181  -1.9748    3.48355  H
 N-N--0.516300         0    -8.09524  -6.50994   5.14543  L
 C-CT-0.038100        -1    -8.33869  -7.95567   5.23186  L
 C-C-0.536600          0    -9.48106  -8.44798   4.32097  L
 O-O--0.581900         0    -10.6696  -8.31434   4.59549  L
 C-CT--0.030300        0    -8.54645  -8.40604   6.69005  L
 C-C-0.799400          0    -9.74528  -7.77271   7.3921   L
 O-O2--0.801400        0    -10.02631  -6.58188   7.13551  L
 O-O2--0.801400        0    -10.35484  -8.44339   8.25482  L
 H-H-0.293600          0    -8.68021  -5.9543    5.76138  L
 H-H1-0.088000         0    -7.43136  -8.4624    4.90123  L
 H-HC--0.012200        0    -7.65705  -8.17032   7.27015  L
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H-HC--0.012200       0    -8.66116  -9.4915    6.69864  L
N-N--0.415700        0    -9.09261  -9.07109   3.21351  L
C-CT--0.038900       -1   -9.95447  -9.60771   2.14281  L
C-C-0.597300         0    -9.40731  -10.91668   1.55814  L
O-O--0.567900        0    -10.04338  -11.52544   0.69541  L
C-CT-0.365400        0    -10.08406  -8.56185   1.01378  L
O-OH--0.676100       0    -8.81731  -8.11846   0.56894  L
C-CT--0.243800       0    -10.84028  -7.30411   1.43975  L
H-H-0.271900         0    -8.09941  -9.01858   3.0224   L
H-H1-0.100700        0    -10.946   -9.81551   2.54299  L
H-H1-0.004300        0    -10.62054  -9.0059    0.17442  L
H-HC-0.064200        0    -10.2641  -6.75839   2.18682  L
H-HC-0.064200        0    -11.80652  -7.57103   1.86602  L
H-HC-0.064200        0    -10.98468  -6.65213   0.57888  L
H-HO-0.410200        0    -8.5782   -8.69007  -0.20646  L
N-N--0.516300        0    -8.2424   -11.3678   2.0353   L
C-CT-0.038100        -1   -7.43463  -12.45589   1.48587  L
C-C-0.536600         0    -7.0806   -13.50517   2.57295  L
N-N--0.415700        0    -8.10802  -14.13284   3.16344  L
C-CT--0.149000       -1   -7.98224  -15.14787   4.21749  L
O-O--0.581900        0    -5.91772  -13.75514   2.89148  L
C-CT--0.030300       0    -6.20756  -11.82892   0.79762  L
C-C-0.799400         0    -5.59975  -12.75479  -0.24624  L
O-O2--0.801400       0    -4.36244  -12.94489  -0.2443   L
O-O2--0.801400       0    -6.37327  -13.20162  -1.12478  L
H-H-0.293600         0    -7.76568  -10.76609   2.69193  L
H-H-0.271900         0    -9.03045  -13.84944   2.87025  L
H-H1-0.088000        0    -8.01891  -12.9763   0.72796  L
H-HC--0.012200       0    -5.46064  -11.54598   1.54173  L
H-HC--0.012200       0    -6.51569  -10.92179   0.27527  L
H-H1-0.097600        0    -7.42617  -16.00748   3.83824  L
H-H1-0.097600        0    -8.96926  -15.47684   4.54586  L
H-H1-0.097600        0    -7.44251  -14.73005   5.06953  L
N-N--0.347900        0    -3.39348  -14.49603   1.96863  L
C-CT--0.263700       -1   -2.23066  -14.87642   2.78978  L
C-C-0.734100         0    -2.20169  -14.06633   4.11224  L
N-N--0.415700        0    -3.37509  -13.86476   4.73616  L
C-CT--0.149000       -1   -3.57583  -13.19785   6.03209  L
O-O--0.589400        0    -1.14123  -13.64057   4.56345  L
C-CT--0.000700       0    -0.94566  -14.72343   1.95002  L
C-CT-0.039000        0    -0.9766   -15.55189   0.64245  L
C-CT-0.048600        0    -0.71283  -14.72031  -0.62052  L
N-N2--0.529500       0    -1.65094  -13.58643  -0.76929  L
C-CA-0.807600        0    -1.34737  -12.35424  -1.12385  L
N-N2--0.862700       0    -0.1614   -12.00915  -1.50889  L
N-N2--0.862700       0    -2.25281  -11.42951  -1.10156  L
H-H-0.271900         0    -4.19991  -14.15738   4.22967  L
H-H-0.274700         0    -3.2963   -13.91029   1.14237  L
H-H-0.274700         0    -4.34039  -14.56789   2.33577  L
H-H1-0.156000        0    -2.32219  -15.92439   3.07609  L
H-HC-0.032700        0    -0.09464  -15.0583   2.54576  L
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H-HC-0.032700        0    -0.78831  -13.66583   1.73131  L
H-HC-0.028500        0    -1.93225  -16.06361   0.52595  L
H-HC-0.028500        0    -0.21036  -16.32562   0.70507  L
H-H1-0.068700        0    -0.79743  -15.36954  -1.49456  L
H-H1-0.068700        0     0.31563  -14.35797  -0.57393  L
H-H-0.345600         0    -2.64919  -13.7244  -0.6379   L
H-H-0.447800         0    -0.07018  -11.10503  -1.95232  L
H-H-0.447800         0     0.39359  -12.77622  -1.87244  L
H-H-0.447800         0    -2.03503  -10.52555  -1.50118  L
H-H-0.447800         0    -3.1807   -11.73025  -0.81054  L
H-H1-0.097600        0    -4.47157  -13.58544   6.51863  L
H-H1-0.097600        0    -3.68826  -12.12314   5.87674  L
H-H1-0.097600        0    -2.71296  -13.36772   6.67931  L
N-N--0.415700        0    -0.22436  -8.89971   11.54906  L
C-CT--0.149000      -1    -0.1123   -8.03648   10.36692  L
C-C-0.597300         0    -1.03364  -6.82307   10.54095  L
N-N--0.415700        0    -2.3457   -7.06109   10.60096  L
C-CT--0.149000       0    -3.35242  -6.06448   10.954   L
O-O--0.567900        0    -0.54947  -5.70992   10.744   L
C-CT--0.015200       0    -0.29392  -8.89122   9.10772  L
C-CA--0.001100       0     0.45642  -10.22041   9.10648  L
C-CA--0.190600       0     1.74301  -10.33252   9.67951  L
C-CA--0.190600       0    -0.1423   -11.35807   8.52905  L
C-CA--0.234100       0     2.41479  -11.5696   9.69816  L
C-CA--0.234100       0     0.53692  -12.59115   8.52149  L
C-C-0.322600         0     1.81102  -12.70368   9.1136   L
O-OH--0.557900       0     2.4573   -13.89701   9.10194  L
H-H-0.271900         0    -2.62792  -8.02096   10.47035  L
H-H-0.271900         0    -0.02627  -9.88961   11.44765  L
H-H-0.271900         0    -0.41538  -8.50675   12.46213  L
H-H1-0.087600        0     0.9048   -7.64365   10.34073  L
H-HC-0.029500        0     0.05137  -8.30999   8.25385  L
H-HC-0.029500        0    -1.35449  -9.10626   8.99098  L
H-HA-0.169900        0     2.23243  -9.46703   10.10532  L
H-HA-0.169900        0    -1.12582  -11.2994   8.0818   L
H-HA-0.165600        0     3.39782  -11.64178   10.14037  L
H-HA-0.165600        0     0.09272  -13.46561   8.0668   L
H-HO-0.399200        0     3.26731  -13.88793   9.61219  L
H-H1-0.097600        0    -3.32279  -5.24485   10.23616  L
H-H1-0.097600        0    -3.14648  -5.66479   11.94876  L
H-H1-0.097600        0    -4.34557  -6.51598   10.94944  L
N-N--0.415700        0     1.82961  -4.23135   11.92543  L
C-CT--0.059700      -1     2.22216  -2.98695   11.24676  L
C-C-0.597300         0     2.24937  -1.7826    12.20328  L
N-N--0.415700        0     1.23794  -1.64233   13.0678  L
C-CT--0.149000       0     1.12277  -0.55755   14.04281  L
O-O--0.567900        0     3.18457  -0.98505   12.14391  L
C-CT-0.130300        0     1.30557  -2.77809   10.0024  L
C-CT--0.043000       0     1.79374  -3.50916   8.72338  L
C-CT--0.320400       0     1.149    -1.29579   9.60862  L
C-CT--0.066000       0     2.16064  -4.99446   8.82724  L
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H-H-0.271900         0     0.51801  -2.34867   13.04261  L
H-H-0.271900         0     1.05608  -4.77894   11.54577  L
H-H-0.271900         0     2.34326  -4.56448   12.73098  L
H-H1-0.086900        0     3.24481  -3.09995   10.8906  L
H-HC-0.018700        0     0.30665  -3.14744   10.24214  L
H-HC-0.023600        0     2.66682  -2.99372   8.33809  L
H-HC-0.023600        0     1.01667  -3.4228    7.96274  L
H-HC-0.088200        0     2.1284   -0.84258   9.45133  L
H-HC-0.088200        0     0.613    -0.74801   10.38411  L
H-HC-0.088200        0     0.57149  -1.214     8.68816  L
H-HC-0.018600        0     2.53941  -5.33229   7.86227  L
H-HC-0.018600        0     1.28176  -5.58327   9.07058  L
H-HC-0.018600        0     2.93673  -5.15317   9.57466  L
H-H1-0.097600        0     0.96236   0.39352   13.53211  L
H-H1-0.097600        0     2.04089  -0.47912   14.62979  L
H-H1-0.097600        0     0.28761  -0.74216   14.72033  L
N-N--0.415700        0     5.07614   1.08749   12.79288  L
C-CT--0.051800      -1     4.48787   2.43117   12.79954  L
C-C-0.597300         0     3.91484   2.76206   14.18539  L
N-N--0.415700        0     4.52169   3.7207    14.89471  L
C-CT--0.149000       0     4.09118   4.14697   16.22612  L
O-O--0.567900        0     2.9246    2.16158   14.59195  L
C-CT-0.110200        0     3.35768   2.53137   11.75957  L
C-CT-0.353100        0     3.80359   2.26303   10.31234  L
C-CT--0.412100       0     2.60303   2.34636   9.37325  L
C-CT--0.412100       0     4.87571   3.24372   9.82588  L
H-H-0.271900         0     5.33422   4.16958   14.50185  L
H-H-0.271900         0     4.45228   0.29355   12.64148  L
H-H-0.271900         0     5.97076   0.92276   13.23544  L
H-H1-0.092200        0     5.25853   3.16457   12.56491  L
H-HC-0.045700        0     2.92128   3.52998   11.81283  L
H-HC-0.045700        0     2.57806   1.81142   12.01507  L
H-HC--0.036100       0     4.19829   1.25455   10.24464  L
H-HC-0.100000        0     2.1721    3.34718   9.39573  L
H-HC-0.100000        0     1.84668   1.62629   9.68369  L
H-HC-0.100000        0     2.91997   2.10547   8.35807  L
H-HC-0.100000        0     5.10461   3.04533   8.78206  L
H-HC-0.100000        0     5.79521   3.11474   10.39508  L
H-HC-0.100000        0     4.5248    4.27163   9.92514  L
H-H1-0.097600        0     4.74032   4.94058   16.60048  L
H-H1-0.097600        0     4.12808   3.30179   16.91704  L
H-H1-0.097600        0     3.06402   4.51558   16.18567  L
N-N--0.415700        0   -12.40455   0.35703   9.28545  L
C-CT--0.001400      -1   -11.28819   0.01893   10.17762  L
C-C-0.597300         0   -10.40281  -1.09483   9.60129  L
O-O--0.567900        0   -9.19713  -0.92772   9.40794  L
C-CT--0.015200       0   -11.82254  -0.32317   11.57635  L
C-CA--0.001100       0   -12.59197   0.81573   12.21947  L
C-CA--0.190600       0   -11.89549   1.93286   12.72084  L
C-CA--0.190600       0   -13.9996   0.7752    12.28903  L
C-CA--0.234100       0   -12.6041   3.00806   13.28989  L
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C-CA--0.234100       0    -14.71081   1.84881   12.86083  L
C-C-0.322600         0    -14.01153   2.96875   13.36229  L
O-OH--0.557900       0    -14.6843   4.01274   13.91114  L
H-H-0.271900         0    -13.16382   0.92281   9.64419  L
H-H-0.271900         0    -12.37528   0.11738   8.29892  L
H-H1-0.087600        0    -10.65304   0.90113   10.271   L
H-HC-0.029500        0    -10.9788  -0.57527   12.22066  L
H-HC-0.029500        0    -12.46488  -1.20306   11.51582  L
H-HA-0.169900        0    -10.81555   1.96963   12.67297  L
H-HA-0.169900        0    -14.5412  -0.07987   11.90781  L
H-HA-0.165600        0    -12.08724   3.87049   13.68369  L
H-HA-0.165600        0    -15.78857   1.8167    12.9165  L
H-HO-0.399200        0    -15.62201   3.83544   13.99804  L
N-N--0.347900        0    -11.05522  -2.216     9.30152  L
C-CT--0.263700      -1    -10.58972  -3.38972   8.55854  L
C-C-0.734100         0    -11.68906  -3.71449   7.54551  L
O-O--0.589400        0    -12.84726  -3.37254   7.79218  L
C-CT--0.000700       0    -10.23283  -4.49726   9.57464  L
C-CT-0.039000        0    -11.37713  -5.11216   10.40823  L
C-CT-0.048600        0    -12.33065  -6.03409   9.6311   L
N-N2--0.529500       0    -13.16122  -6.85491   10.53329  L
C-CA-0.807600        0    -13.08179  -8.15916   10.73768  L
N-N2--0.862700       0    -12.21285  -8.93271   10.15602  L
N-N2--0.862700       0    -13.90844  -8.73324   11.56659  L
H-H-0.274700         0    -12.05902  -2.17511   9.42698  L
H-H1-0.156000        0    -9.69439  -3.12508   8.0074   L
H-HC-0.032700        0    -9.5226   -4.06293   10.28041  L
H-HC-0.032700        0    -9.68556  -5.29189   9.08096  L
H-HC-0.028500        0    -11.9527  -4.3193    10.88669  L
H-HC-0.028500        0    -10.9113  -5.70571   11.19623  L
H-H1-0.068700        0    -11.75085  -6.66561   8.96702  L
H-H1-0.068700        0    -12.99834  -5.43847   9.01265  L
H-H-0.345600         0    -13.89576  -6.36867   11.01462  L
H-H-0.447800         0    -12.15935  -9.91554   10.31508  L
H-H-0.447800         0    -11.55442  -8.54439   9.46498  L
H-H-0.447800         0    -13.84066  -9.72194   11.71507  L
H-H-0.447800         0    -14.60715  -8.19492   12.04403  L
N-N--0.415700        0    -11.34524  -4.30223   6.4117   L
C-CT--0.003100      -1    -12.27533  -4.53079   5.30469  L
C-C-0.597300         0    -13.16262  -5.7865    5.46997  L
N-N--0.415700        0    -12.76776  -6.75873   6.30189  L
C-CT--0.149000      -1    -13.52815  -7.97253   6.60332  L
O-O--0.567900        0    -14.22143  -5.86581   4.84667  L
C-CT--0.003600       0    -11.50773  -4.567     3.97331  L
C-CT--0.064500       0    -10.9902  -3.16254   3.63153  L
C-C-0.695100         0    -10.34998  -3.05634   2.25345  L
O-O--0.608600        0    -9.62951  -3.93      1.78278  L
N-N--0.940700        0    -10.55548  -1.94823   1.58175  L
H-H-0.271900         0    -10.43647  -4.7477    6.4005   L
H-H-0.271900         0    -11.8183  -6.67733   6.66293  L
H-H1-0.085000        0    -12.9709  -3.69012   5.25847  L
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H-HC-0.017100        0    -12.18204  -4.89009   3.17874  L
H-HC-0.017100        0    -10.67641  -5.27013   4.0414   L
H-HC-0.035200        0    -10.25051  -2.85593   4.3705   L
H-HC-0.035200        0    -11.82551  -2.46247   3.68039  L
H-H-0.425100         0    -9.78061  -1.71339   0.96938  L
H-H-0.425100         0    -11.13747  -1.22925   1.98664  L
H-H1-0.097600        0    -12.91907  -8.63911   7.21534  L
H-H1-0.097600        0    -13.7805  -8.47975   5.67102  L
H-H1-0.097600        0    -14.44611  -7.71291   7.13139  L
N-N--0.347900        0    -14.81545  -14.79116  -4.35761  L
C-CT--0.240000       -1   -14.78295  -13.32004  -4.37394  L
C-C-0.734100         0    -15.53116  -12.7515  -5.60878  L
N-N-0.415700         0    -15.93666  -11.47808  -5.6801   L
C-CT-0.149000        0    -15.879   -10.43803  -4.66157  L
O-O--0.589400        0    -15.74035  -13.48688  -6.56195  L
C-CT--0.009400       0    -13.29685  -12.851   -4.39487  L
C-CT-0.018700        0    -12.42187  -13.19495  -3.16363  L
C-CT--0.047900       0    -11.03529  -12.50123  -3.21329  L
C-CT--0.014300       0    -10.06722  -13.01101  -2.12431  L
N-N3--0.385400       0    -8.77239  -12.27488  -2.09879  L
H-H-0.274700         0    -16.36565  -11.2708  -6.56938  L
H-H-0.271900         0    -14.56019  -15.32317  -3.53146  L
H-H-0.271900         0    -15.04868  -15.29714  -5.21069  L
H-H1-0.142600        0    -15.25985  -12.96643  -3.4576   L
H-HC-0.036200        0    -13.28268  -11.77095  -4.50797  L
H-HC-0.036200        0    -12.81253  -13.26803  -5.28099  L
H-HC-0.010300        0    -12.27837  -14.27564  -3.12471  L
H-HC-0.010300        0    -12.93858  -12.87981  -2.25595  L
H-HC-0.062100        0    -11.17159  -11.42539  -3.09023  L
H-HC-0.062100        0    -10.58096  -12.68194  -4.18934  L
H-HP-0.113500        0    -9.87146  -14.07219  -2.30188  L
H-HP-0.113500        0    -10.5455  -12.91735  -1.14442  L
H-H-0.340000         0    -8.33574  -12.16833  -3.00394  L
H-H-0.340000         0    -8.05833  -12.75396  -1.54376  L
H-H-0.340000         0    -8.84446  -11.33987  -1.69109  L
H-H1-0.097600        0    -15.45047  -10.81011  -3.73206  L
H-H1-0.097600        0    -16.88547  -10.07055  -4.45412  L
H-H1-0.097600        0    -15.27377  -9.60566  -5.02243  L
N-N--0.254800        0    -15.65026  -9.13442  -1.49569  L
C-CT--0.026600       -1   -14.70222  -8.07762  -1.82705  L
C-C-0.589600         0    -13.55361  -8.57923  -2.71057  L
O-O--0.574800        0    -13.32277  -9.77955  -2.87429  L
C-CT--0.007000       0    -14.21412  -7.53134  -0.4767   L
C-CT-0.018900        0    -14.44166  -8.68514   0.50232  L
C-CT-0.019200        0    -15.68946  -9.36373  -0.06267  L
H-H1-0.064100        0    -15.22639  -7.28239  -2.35855  L
H-HC-0.025300        0    -14.83852  -6.68522  -0.18362  L
H-HC-0.025300        0    -13.167   -7.22858  -0.50304  L
H-HC-0.021300        0    -14.60432  -8.32465   1.51904  L
H-HC-0.215300        0    -13.59727  -9.37594   0.47641  L
H-H1-0.039100        0    -15.68576  -10.42989   0.16683  L
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H-H1-0.039100        0    -16.58381  -8.89541   0.35197  L
N-N--0.415700        0    -12.87299  -7.63719  -3.35118  L
C-CT--0.038900       -1   -11.65219  -7.76325  -4.16944  L
C-C-0.597300         0    -11.06225  -6.35849  -4.17551  L
O-O--0.567900        0    -11.8264  -5.40369  -4.33124  L
C-CT-0.365400        0    -11.97412  -8.24015  -5.59807  L
O-OH--0.676100       0    -12.76587  -9.4129   -5.52332  L
C-CT--0.243800       0    -10.71097  -8.59631  -6.37632  L
H-H-0.271900         0    -13.15789  -6.67753  -3.19521  L
H-H1-0.100700        0    -10.94735  -8.44988  -3.69604  L
H-H1-0.004300        0    -12.5292  -7.46868  -6.13339  L
H-HC-0.064200        0    -10.08186  -7.71402  -6.49536  L
H-HC-0.064200        0    -10.9836  -8.96624  -7.365    L
H-HC-0.064200        0    -10.14717  -9.36645  -5.84836  L
H-HO-0.410200        0    -12.63143  -9.72568  -4.61477  L
N-N--0.415700        0    -9.76652  -6.21041  -3.91727  L
C-CT--0.001400       -1   -9.10929  -4.93418  -3.60905  L
C-C-0.597300         0    -9.528    -3.78097  -4.53214  L
O-O--0.567900        0    -10.03491  -2.78626  -4.02891  L
C-CT--0.015200       0    -7.60282  -5.16675  -3.60935  L
C-CA--0.001100       0    -6.78655  -3.90351  -3.77782  L
C-CA--0.190600       0    -6.23989  -3.60665  -5.03897  L
C-CA--0.190600       0    -6.65028  -2.99022  -2.71547  L
C-CA--0.234100       0    -5.60511  -2.37701  -5.25758  L
C-CA--0.234100       0    -6.01898  -1.75219  -2.93315  L
C-C-0.322600         0    -5.53342  -1.43008  -4.21777  L
O-OH--0.557900       0    -5.03944  -0.19723  -4.48883  L
H-H-0.271900         0    -9.19989  -7.05391  -3.81162  L
H-H1-0.087600        0    -9.38403  -4.63633  -2.59622  L
H-HC-0.029500        0    -7.34926  -5.85575  -4.41573  L
H-HC-0.029500        0    -7.35674  -5.64565  -2.66535  L
H-HA-0.169900        0    -6.3382   -4.30645  -5.85601  L
H-HA-0.169900        0    -7.06153  -3.20843  -1.7359   L
H-HA-0.165600        0    -5.18931  -2.13748  -6.22334  L
H-HA-0.165600        0    -5.95516  -1.03934  -2.12194  L
H-HO-0.399200        0    -4.83494   0.29185  -3.6644   L
N-N--0.415700        0    -9.42114  -3.94296  -5.85975  L
C-CT-0.014300        -1   -9.83344  -2.976    -6.89751  L
C-C-0.597300         0    -11.27564  -2.44465  -6.81416  L
O-O--0.567900        0    -11.61486  -1.51613  -7.53704  L
C-CT--0.204100       0    -9.54733  -3.58667  -8.28434  L
C-C-0.713000         0    -8.08008  -3.5219   -8.66933  L
O-O--0.593100        0    -7.25559  -4.30478  -8.22612  L
N-N--0.919100        0    -7.70181  -2.58933  -9.5099   L
H-H-0.271900         0    -8.93731  -4.77465  -6.16429  L
H-H1-0.104800        0    -9.2066   -2.08964  -6.78714  L
H-HC-0.079700        0    -10.11664  -3.04408  -9.04044  L
H-HC-0.079700        0    -9.87616  -4.62455  -8.31318  L
H-H-0.419600         0    -6.75952  -2.66021  -9.84882  L
H-H-0.419600         0    -8.40763  -1.98442  -9.93105  L
N-N--0.415700        0    -12.10199  -3.00018  -5.93173  L
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C-CT--0.002400       -1   -13.40882  -2.48022  -5.55529  L
C-C-0.597300         0    -13.49232  -2.0985   -4.07648  L
O-O--0.567900        0    -13.9672  -1.01669  -3.74541  L
C-CT--0.034300       0    -14.48019  -3.51326  -5.93114  L
C-CA-0.011800        0    -15.89176  -3.0856   -5.57731  L
C-CA--0.125600       0    -16.59928  -2.22226  -6.43459  L
C-CA--0.125600       0    -16.48816  -3.52129  -4.37716  L
C-CA--0.170400       0    -17.89853  -1.80315  -6.09802  L
C-CA--0.170400       0    -17.78819  -3.10227  -4.04192  L
C-CA--0.107200       0    -18.4933  -2.24348  -4.90304  L
H-H-0.271900         0    -11.71719  -3.75193  -5.3773   L
H-H1-0.097800        0    -13.61585  -1.56893  -6.12108  L
H-HC-0.029500        0    -14.26096  -4.45765  -5.43134  L
H-HC-0.029500        0    -14.43112  -3.69172  -7.00655  L
H-HA-0.133000        0    -16.14394  -1.86545  -7.34829  L
H-HA-0.133000        0    -15.9452  -4.16005  -3.69818  L
H-HA-0.143000        0    -18.43672  -1.13094  -6.75282  L
H-HA-0.143000        0    -18.24461  -3.42002  -3.1151   L
H-HA-0.129700        0    -19.488   -1.90807  -4.64188  L
N-N--0.415700        0    -13.02592  -2.9758   -3.18435  L
C-CT-0.033700        -1   -12.99469  -2.73224  -1.74421  L
C-C-0.597300         0    -12.33216  -1.38952  -1.38958  L
O-O--0.567900        0    -12.92119  -0.57565  -0.68127  L
C-CT--0.182500       0    -12.31013  -3.92121  -1.05644  L
H-H-0.271900         0    -12.58608  -3.81103  -3.54479  L
H-H1-0.082300        0    -14.02353  -2.67614  -1.38433  L
H-HC-0.060300        0    -12.82628  -4.84583  -1.30901  L
H-HC-0.060300        0    -12.34399  -3.78042   0.02521  L
H-HC-0.060300        0    -11.26689  -3.98757  -1.36626  L
N-N--0.415700        0    -11.14045  -1.14198  -1.94225  L
C-CT--0.087500       -1   -10.41149   0.12529  -1.8221   L
C-C-0.597300         0    -11.22865   1.32654  -2.27903  L
O-O--0.567900        0    -11.14886   2.3774   -1.66319  L
C-CT-0.298500        0    -9.0485    0.04073  -2.54319  L
C-CT--0.319200       0    -9.11315   0.24116  -4.06276  L
C-CT--0.319200       0    -8.04134   1.0472   -1.98442  L
H-H-0.271900         0    -10.7425  -1.8542   -2.54455  L
H-H1-0.096900        0    -10.20787   0.27679  -0.76134  L
H-HC--0.029700       0    -8.64332  -0.9531   -2.35761  L
H-HC-0.079100        0    -8.16653  -0.07423  -4.49574  L
H-HC-0.079100        0    -9.28511   1.2918   -4.30224  L
H-HC-0.079100        0    -9.91069  -0.3566   -4.4955   L
H-HC-0.079100        0    -7.79795   0.77944  -0.95844  L
H-HC-0.079100        0    -8.4578    2.05358  -2.01637  L
H-HC-0.079100        0    -7.12422   1.02296  -2.57044  L
N-N--0.415700        0    -12.01614   1.17846  -3.34588  L
C-CT--0.087500       -1   -12.81008   2.25745  -3.94064  L
C-C-0.597300         0    -13.94399   2.69691  -3.02411  L
O-O--0.567900        0    -14.1112   3.8888   -2.77968  L
C-CT-0.298500        0    -13.33754   1.89005  -5.34396  L
C-CT--0.319200       0    -14.02259   3.08356  -6.02088  L
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C-CT--0.319200       0    -12.19332   1.44055  -6.26096  L
H-H-0.271900         0    -12.0955   0.25341  -3.73795  L
H-H1-0.096900        0    -12.15665   3.12345  -4.05554  L
H-HC--0.029700       0    -14.05912   1.07804  -5.26683  L
H-HC-0.079100        0    -14.33821   2.80803  -7.02814  L
H-HC-0.079100        0    -13.33227   3.92525  -6.08721  L
H-HC-0.079100        0    -14.90458   3.38667  -5.45704  L
H-HC-0.079100        0    -11.72471   0.54041  -5.87153  L
H-HC-0.079100        0    -11.44997   2.23334  -6.34223  L
H-HC-0.079100        0    -12.5857   1.21404  -7.25292  L
N-N--0.415700        0    -14.71289   1.73898  -2.50243  L
C-CT--0.087500       -1   -15.74876   1.99929  -1.49191  L
C-C-0.597300         0    -15.15201   2.70077  -0.27805  L
O-O--0.567900        0    -15.61661   3.76259   0.12537  L
C-CT-0.298500        0    -16.47963   0.69881  -1.0959   L
C-CT--0.319200       0    -17.56129   0.94844  -0.03617  L
C-CT--0.319200       0    -17.16873   0.05718  -2.30919  L
H-H-0.271900         0    -14.49466   0.78358  -2.76288  L
H-H1-0.096900        0    -16.48132   2.68264  -1.92139  L
H-HC--0.029700       0    -15.75937  -0.01465  -0.69395  L
H-HC-0.079100        0    -18.08685   0.01972   0.18537  L
H-HC-0.079100        0    -18.27529   1.68972  -0.39664  L
H-HC-0.079100        0    -17.1084   1.3082    0.88804  L
H-HC-0.079100        0    -17.87896   0.75716  -2.75006  L
H-HC-0.079100        0    -17.69738  -0.84397  -2.00099  L
H-HC-0.079100        0    -16.43304  -0.22255  -3.06243  L
N-N--0.516300        0    -14.12687   2.09415   0.30566  L
C-CT-0.038100        -1   -13.51446   2.50009   1.56643  L
C-C-0.536600         0    -12.69044   3.79349   1.46222  L
O-O--0.581900        0    -12.61325   4.55257   2.42039  L
C-CT--0.030300       0    -12.7096   1.28155   2.04272  L
C-C-0.799400         0    -12.54545   1.21891   3.55439  L
O-O2--0.801400       0    -12.17378   2.25229   4.14673  L
O-O2--0.801400       0    -12.67733   0.10495   4.10569  L
H-H-0.293600         0    -13.78561   1.23657  -0.11555  L
H-H1-0.088000        0    -14.31039   2.68244   2.29     L
H-HC--0.012200       0    -11.73498   1.26842   1.55406  L
H-HC--0.012200       0    -13.23521   0.37097   1.74768  L
N-N--0.516300        0    -12.1117   4.11913   0.30521  L
C-CT-0.038100        -1   -11.47058   5.42196   0.0933   L
C-C-0.536600         0    -12.44094   6.60272  -0.04254  L
O-O--0.581900        0    -12.00633   7.74946   0.06575  L
C-CT--0.030300       0    -10.40978   5.37878  -1.02962  L
C-C-0.799400         0    -9.09076   4.71097  -0.59561  L
O-O2--0.801400       0    -8.91557   4.38254   0.60075  L
O-O2--0.801400       0    -8.15134   4.59077  -1.41704  L
H-H-0.293600         0    -12.12608   3.45442  -0.46225  L
H-H1-0.088000        0    -10.92316   5.65922   1.00573  L
H-HC--0.012200       0    -10.16489   6.40296  -1.31537  L
H-HC--0.012200       0    -10.81821   4.88836  -1.91306  L
N-N--0.415700        0    -13.74794   6.35619  -0.16361  L
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C-CT--0.058100       -1   -14.78279   7.39621  -0.16224  L
C-C-0.597300         0    -15.74328   7.22271   1.02031  L
N-N--0.415700        0    -16.6411   6.2364    0.97492  L
C-CT--0.149000       0    -17.61176   5.92802   2.02176  L
O-O--0.567900        0    -15.64029   7.96198   2.00202  L
C-CT--0.007400       0    -15.46458   7.45772  -1.53469  L
C-CC-0.186800        0    -14.52603   7.9821   -2.5924   L
N-NB--0.543200       0    -14.11088   9.30927  -2.70625  L
C-CW--0.220700       0    -13.88463   7.23094  -3.53235  L
C-CR-0.163500        0    -13.23348   9.32972  -3.71997  L
N-NA--0.279500       0    -13.07665   8.09715  -4.23672  L
H-H-0.271900         0    -14.0212   5.38257  -0.24054  L
H-H-0.271900         0    -16.52502   5.56388   0.22345  L
H-H1-0.136000        0    -14.31631   8.3705   -0.0137   L
H-HC-0.036700        0    -16.3208   8.13061  -1.47883  L
H-HC-0.036700        0    -15.81996   6.46609  -1.81968  L
H-H4-0.186200        0    -13.98133   6.16232  -3.66334  L
H-H-0.333900         0    -12.45998   7.8535   -4.99963  L
H-H5-0.143500        0    -12.72218   10.21761  -4.06697  L
H-H1-0.097600        0    -18.08961   6.84509   2.37139  L
H-H1-0.097600        0    -17.10735   5.44171   2.85802  L
H-H1-0.097600        0    -18.37438   5.25418   1.62834  L
N-N--0.415700        0    -13.98145   6.37545   3.92611  L
C-CT--0.023700       -1   -13.1522   7.05693   4.91993  L
C-C-0.597300         0    -12.96494   8.57477   4.66667  L
N-N--0.415700        0    -13.66357   9.16027   3.68845  L
C-CT--0.149000       0    -13.76027   10.59871   3.45493  L
O-O--0.567800        0    -12.23124   9.2464    5.40563  L
C-CT-0.034200        0    -11.80283   6.34398   5.1119   L
C-CT-0.001800        0    -11.96309   5.04476   5.9011   L
S-S--0.273700        0    -10.39125   4.34846   6.47722  L
C-CT--0.053600       0    -11.0207   2.87176   7.3172   L
H-H-0.271900         0    -14.24905   8.56605   3.10651  L
H-H-0.271900         0    -13.59464   5.54434   3.47787  L
H-H-0.271900         0    -14.79819   6.81256   3.51021  L
H-H1-0.088000        0    -13.68406   6.99508   5.86911  L
H-HC-0.024100        0    -11.143    6.98477   5.69453  L
H-HC-0.024100        0    -11.33105   6.1462    4.14844  L
H-H1-0.044000        0    -12.48212   4.31943   5.27886  L
H-H1-0.044000        0    -12.58159   5.23753   6.77749  L
H-H1-0.068400        0    -11.6728   3.16848   8.13789  L
H-H1-0.068400        0    -10.18552   2.2908    7.70769  L
H-H1-0.068400        0    -11.58677   2.26297   6.61095  L
H-H1-0.097600        0    -12.76724   11.04632   3.44086  L
H-H1-0.097600        0    -14.36028   11.06022   4.24088  L
H-H1-0.097600        0    -14.24833   10.77486   2.49367  L
N-N--0.415700        0    -11.68586   10.36601   1.01424  L
C-CT--0.059700       -1   -10.32359   10.79321   1.34154  L
C-C-0.597300         0    -9.96909   11.99073   0.43689  L
N-N--0.415700        0    -10.09198   13.207    0.98187  L
C-CT--0.149000       0    -9.8232    14.47478   0.30203  L
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O-O--0.567900        0    -9.61502   11.83167  -0.73052  L
C-CT-0.130300        0    -9.35717   9.59417   1.1594    L
C-CT--0.043000       0    -9.59828   8.48349   2.21228   L
C-CT--0.320400       0    -7.86939   9.98887   1.14594   L
C-CT--0.066000       0    -9.31612   8.8642    3.67331   L
H-H-0.271900         0    -10.41463   13.24082   1.93251  L
H-H-0.271900         0    -11.82814   9.36056   0.89983   L
H-H-0.271900         0    -12.21447   10.93664   0.3656   L
H-H1-0.086900        0    -10.28399   11.12803   2.37483  L
H-HC-0.018700        0    -9.56478   9.15732   0.18016   L
H-HC-0.023600        0    -8.98107   7.62203   1.95492   L
H-HC-0.023600        0    -10.6339   8.15233   2.15832   L
H-HC-0.088200        0    -7.27442   9.12359   0.86856   L
H-HC-0.088200        0    -7.55067   10.37577   2.11055  L
H-HC-0.088200        0    -7.67202   10.74374   0.39184  L
H-HC-0.018600        0    -9.95278   9.68949   3.98665   L
H-HC-0.018600        0    -8.27294   9.137     3.81061   L
H-HC-0.018600        0    -9.52585   8.00325   4.30295   L
H-H1-0.097600        0    -10.5395   15.23235   0.6236   L
H-H1-0.097600        0    -9.91415   14.35293  -0.78029  L
H-H1-0.097600        0    -8.81265   14.81546   0.53434  L
N-N--0.415703        0    -7.02729   13.09299  -0.94987  L
C-CT--0.058100      -1    -5.6449    12.76972  -1.29632  L
C-C-0.597300         0    -5.39719   11.25902  -1.2439   L
O-O--0.567900        0    -4.90733   10.70132  -0.25631  L
C-CT--0.007400       0    -4.71573   13.54777  -0.34483  L
C-CC-0.186800        0    -4.98305   15.03297  -0.2854   L
N-NB--0.543200       0    -5.96418   15.6516   0.49876   L
C-CW--0.220700       0    -4.31278   15.98326  -0.99645  L
C-CR-0.163500        0    -5.86101   16.96388   0.23488  L
N-NA--0.279500       0    -4.87901   17.19278  -0.65572  L
H-H-0.271900         0    -7.14843   13.7847  -0.21618  L
H-H-0.271900         0    -7.8086    12.47696  -1.16878  L
H-H1-0.136000        0    -5.44263   13.11515  -2.31031  L
H-HC-0.036700        0    -3.6794    13.38439  -0.63883  L
H-HC-0.036700        0    -4.83589   13.16174   0.66183  L
H-H4-0.186200        0    -3.4979    15.80754  -1.68523  L
H-H-0.333900         0    -4.61007   18.10306  -1.00699  L
H-H5-0.143500        0    -6.48182   17.7335   0.67562   L
N-N--0.415700        0    -5.76389   10.57912  -2.33105  L
C-CT--0.087500      -1    -5.71268   9.11423  -2.4458   L
C-C-0.597300         0    -4.29088   8.66093  -2.78801  L
O-O--0.567900        0    -3.97437   8.23996  -3.89907  L
C-CT-0.298500        0    -6.78156   8.60212  -3.44077  L
C-CT--0.319200       0    -6.98319   7.09515  -3.27446  L
C-CT--0.319200       0    -8.1564    9.25086  -3.20615  L
H-H-0.271900         0    -6.20577   11.09307  -3.07864  L
H-H1-0.096900        0    -5.97034   8.69764  -1.47795  L
H-HC--0.029700       0    -6.47433   8.82574  -4.46072  L
H-HC-0.079100        0    -6.05167   6.55731  -3.44507  L
H-HC-0.079100        0    -7.72567   6.7407   -3.98969  L
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 H-HC-0.079100        0    -7.3571    6.88421  -2.27506  L
 H-HC-0.079100        0    -8.47443   9.10819  -2.17261  L
 H-HC-0.079100        0    -8.89468   8.79226  -3.86615  L
 H-HC-0.079100        0    -8.13006   10.31527  -3.43355  L
 N-N--0.415700        0    -3.39385   8.85059  -1.82625  L
 C-CT--0.002400       -1   -1.95423   8.72171  -2.01376  L
 C-C-0.597300         0    -1.46772   7.30529  -1.68194  L
 O-O--0.567900        0    -1.98807   6.64486  -0.7761   L
 C-CT--0.034300       0    -1.2287    9.76783  -1.15402  L
 C-CA-0.011800        0    -1.30566   11.22888  -1.58542  L
 C-CA--0.125600       0    -2.14394   11.68204  -2.62941  L
 C-CA--0.125600       0    -0.46371   12.15258  -0.93743  L
 C-CA--0.170400       0    -2.12926   13.03311  -3.02064  L
 C-CA--0.170400       0    -0.45453   13.5046  -1.3218   L
 C-CA--0.107200       0    -1.28162   13.9443  -2.36861  L
 H-H-0.271900         0    -3.72802   9.27203  -0.96867  L
 H-H1-0.097800        0    -1.70331   8.91382  -3.0579   L
 H-HC-0.029500        0    -0.16998   9.50357  -1.13936  L
 H-HC-0.029500        0    -1.59375   9.69136  -0.1294   L
 H-HA-0.133000        0    -2.77706   11.00605  -3.17828  L
 H-HA-0.133000        0     0.20088   11.81758  -0.15134  L
 H-HA-0.143000        0    -2.73841   13.36615  -3.85005  L
 H-HA-0.143000        0     0.21331   14.1988  -0.82979  L
 H-HA-0.129700        0    -1.24288   14.97689  -2.68687  L
 N-N--0.347900        0    -0.46898   6.83854  -2.43731  L
 C-CT--0.263700       -1    0.14449   5.50374  -2.37075  L
 C-C-0.734100         0     1.40207   5.41056  -3.2343   L
 O-O--0.589400        0     1.89814   6.43621  -3.68725  L
 C-CT--0.000700       0    -0.89943   4.45369  -2.80712  L
 C-CT-0.039000        0    -1.51809   4.65134  -4.19634  L    H-H1
1046  0.        0.
 C-CT-0.048600        0    -2.62769   3.61425  -4.34593  H
 N-N2--0.529500       0    -3.30281   3.76001  -5.62681  H
 C-CA-0.807600        0    -4.55585   3.35593  -5.80171  H
 N-N2--0.862700       0    -5.24216   2.82535  -4.79811  H
 N-N2--0.862700       0    -5.12591   3.46847  -7.01817  H
 H-H-0.274700         0    -0.15086   7.42881  -3.20369  L
 H-H1-0.156000        0     0.44307   5.28785  -1.3448   L
 H-HC-0.032700        0    -1.69653   4.45142  -2.07157  L
 H-HC-0.032700        0    -0.45842   3.46063  -2.78746  L
 H-HC-0.028500        0    -0.76163   4.50795  -4.96895  L
 H-HC-0.028500        0    -1.94951   5.64911  -4.28615  L
 H-H1-0.068700        0    -3.35841   3.78022  -3.55061  H
 H-H1-0.068700        0    -2.22135   2.60682  -4.22037  H
 H-H-0.345600         0    -2.76416   3.91262  -6.46736  H
 H-H-0.447800         0    -6.21047   2.58442  -5.02292  H
 H-H-0.447800         0    -4.81132   2.35988  -3.98411  H
 H-H-0.447800         0    -6.10723   3.1966   -7.05674  H
 H-H-0.447800         0    -4.84346   4.18794  -7.67416  H
 N-N--0.415700        0     1.90624   4.20108  -3.47182  L
 C-CT--0.025200       -1    3.05566   3.91576  -4.32677  L
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 C-C-0.597300          0     2.72301   3.75052  -5.8088   L
 O-O--0.567900         0     1.58846   3.50264  -6.22271  L
 H-H-0.271900          0     1.4253    3.39617  -3.08331  L
 H-H1-0.069800         0     3.51056   2.98491  -3.99056  L
 H-H1-0.069800         0     3.78821   4.71135  -4.20752  L
 N-N--0.516300         0     3.7764    3.86179  -6.60727  L
 C-CT-0.039700         0     3.86581   3.58687  -8.04329  L
 C-C-0.536600          0     3.35087   2.18762  -8.41875  L
 O-O--0.581900         0     2.72947   2.02072  -9.46826  L
 C-CT-0.056000         0     5.33217   3.81221  -8.41905  L
 C-CT-0.013600         0     5.71169   3.58125  -9.8819   L
 C-C-0.805400          0     7.14594   4.07606  -10.11501  L
 O-O2--0.818800        0     8.07659   3.61042  -9.41693  L
 O-O2--0.818800        0     7.35767   4.97378  -10.95692  L
 H-H-0.293600          0     4.63184   4.17547  -6.15735  L
 H-H1-0.110500         0     3.26678   4.3137   -8.59064  L
 H-HC--0.017300        0     5.95996   3.17925  -7.78911  L
 H-HC--0.017300        0     5.55014   4.85331  -8.1868   L
 H-HC--0.042500        0     5.01491   4.12664  -10.5228  L
 H-HC--0.042500        0     5.64357   2.51625  -10.11387  L
 N-N--0.516300         0     3.52211   1.19481  -7.53586  L
 C-CT-0.038100        -1     2.97577  -0.16142  -7.68713  L
 C-C-0.536600          0     1.43971  -0.21276  -7.87386  L
 O-O--0.581900         0     0.92279  -1.21298  -8.37888  L
 C-CT--0.030300        0     3.49182  -1.0874   -6.57408  L
 C-C-0.799400          0     2.77801  -0.97739  -5.23069  L
 O-O2--0.801400        0     2.4777    0.14889  -4.78288  L
 O-O2--0.801400        0     2.60289  -2.0486   -4.59972  L
 H-H-0.293600          0     3.95855   1.42767  -6.6558   L
 H-H1-0.088000         0     3.39165  -0.54911  -8.61762  L
 H-HC--0.012200        0     4.54936  -0.9034   -6.40506  L
 H-HC--0.012200        0     3.40727  -2.11358  -6.92909  L
 N-N--0.415700         0     0.71975   0.87345  -7.55715  L
 C-CT--0.058100        0    -0.72314   1.05004  -7.78031  L    H-HC
1102  0.        0.
 C-C-0.597300          0    -1.09646   2.25535  -8.6678   L
 O-O--0.567900         0    -2.27245   2.6243   -8.75414  L
 C-CT--0.007400        0    -1.41841   1.08869  -6.41518  H
 C-CC-0.186800         0    -1.53452  -0.25071  -5.76554  H
 N-NB--0.543200        0    -2.47494  -1.14828  -6.2167   H
 C-CW--0.220700        0    -0.81231  -0.79508  -4.73705  H
 C-CR-0.163500         0    -2.32326  -2.20869  -5.45167  H
 N-NA--0.279500        0    -1.32752  -2.05004  -4.55172  H
 H-H-0.271900          0     1.23142   1.61946  -7.09425  L
 H-H1-0.136000         0    -1.10399   0.1758   -8.30782  L
 H-HC-0.036700         0    -2.441     1.45519  -6.55641  H
 H-HC-0.036700         0    -0.87878   1.79663  -5.77597  H
 H-H4-0.186200         0     0.01273  -0.4258   -4.14705  H
 H-H-0.333900          0    -1.10364  -2.669    -3.77058  H
 H-H5-0.143500         0    -2.90894  -3.11804  -5.49618  H
 N-N--0.415700         0    -0.14746   2.81988  -9.42294  L
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C-CT--0.051800       -1   -0.43988   3.68461  -10.57918  L
C-C-0.597300         0    -1.30988   2.92834  -11.58932  L
O-O--0.567900        0    -2.43707   3.32007  -11.88023  L
C-CT--0.110200       0     0.89106   4.16991  -11.19157  L
C-CT-0.353100        0     0.75354   5.00606  -12.47867  L
C-CT--0.412100       0    -0.05186   6.28754  -12.27294  L
C-CT--0.412100       0     2.14329   5.39047  -12.98332  L
H-H-0.271900         0     0.80701   2.48945  -9.29732  L
H-H1-0.092200        0    -1.00626   4.55206  -10.24525  L
H-HC-0.045700        0     1.50812   3.30124  -11.42399  L
H-HC-0.045700        0     1.42604   4.75951  -10.44823  L
H-HC--0.036100       0     0.2662    4.40622  -13.24745  L
H-HC-0.100000        0    -1.06934   6.05609  -11.96242  L
H-HC-0.100000        0    -0.09605   6.84786  -13.20674  L
H-HC-0.100000        0     0.42559   6.90817  -11.51441  L
H-HC-0.100000        0     2.65553   6.00677  -12.24285  L
H-HC-0.100000        0     2.05837   5.95103  -13.9144  L
H-HC-0.100000        0     2.73545   4.49401  -13.16773  L
N-N--0.415700        0    -0.80316   1.78768  -12.05213  L
C-CT--0.024900       -1   -1.44781   0.83221  -12.95996  L
C-C-0.597300         0    -2.9055    0.49115  -12.60148  L
O-O--0.567900        0    -3.74216   0.38921  -13.50073  L
C-CT-0.211700        0    -0.60288  -0.44809  -12.97904  L
O-OH--0.654600       0    -0.51701  -0.9647   -11.66255  L
H-H-0.271900         0     0.1035    1.53771  -11.68084  L
H-H1-0.084300        0    -1.44767   1.25909  -13.96294  L
H-H1-0.035200        0     0.39866  -0.21305  -13.34366  L
H-H1-0.035200        0    -1.05923  -1.18741  -13.63894  L
H-HO-0.427500        0     0.26022  -1.52994  -11.57707  L
N-N--0.415700        0    -3.21488   0.28143  -11.31562  L
C-CT-0.014300        -1   -4.55314  -0.04178  -10.79489  L
C-C-0.597300         0    -5.5185    1.1458   -10.78153  L
O-O--0.567900        0    -6.7237    0.91893  -10.78829  L
C-CT--0.204100       0    -4.40885  -0.72508  -9.4317   L
C-C-0.713000         0    -3.75807  -2.0849   -9.58767  L
O-O--0.593100        0    -4.17458  -2.89827  -10.40541  L
N-N--0.919100        0    -2.73647  -2.37478  -8.82953  L
H-H-0.271900         0    -2.4285    0.30121  -10.68063  L
H-H1-0.104800        0    -5.00997  -0.76173  -11.47617  L
H-HC-0.079700        0    -5.39817  -0.88775  -9.01496  L
H-HC-0.079700        0    -3.83727  -0.09676  -8.74693  L
H-H-0.419600         0    -2.36821  -3.3191   -8.86852  L
H-H-0.419600         0    -2.45801  -1.76908  -8.06312  L
N-N--0.415700        0    -5.01975   2.38407  -10.82113  L
C-CT--0.038900       -1   -5.8286    3.61601  -10.79085  L
C-C-0.597300         0    -6.9604    3.63801  -11.81923  L
O-O--0.567900        0    -8.11302   3.71056  -11.40805  L
C-CT-0.365400        0    -4.95711   4.87074  -10.72037  L
O-OH--0.676100       0    -4.18487   4.74474  -9.53947  L
C-CT--0.243800       0    -5.76688   6.15376  -10.58444  L
H-H-0.271900         0    -4.01391   2.47768  -10.90318  L
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H-H1-0.100700        0    -6.35306   3.59728  -9.83477  L
H-H1-0.004300        0    -4.30812   4.94535  -11.59095  L
H-HC-0.064200        0    -5.09839   6.99929  -10.42519  L
H-HC-0.064200        0    -6.44812   6.07381  -9.73764  L
H-HC-0.064200        0    -6.34625   6.33349  -11.48972  L
H-HO-0.410200        0    -3.51101   4.06539  -9.70328  L
N-N--0.254800        0    -6.72683   3.46409  -13.12835  L
C-CT--0.026600       -1   -7.82291   3.39313  -14.09875  L
C-C-0.589600         0    -8.57007   2.04432  -14.18206  L
O-O--0.574800        0    -9.34998   1.83725  -15.10482  L
C-CT--0.007000       0    -7.14203   3.73524  -15.43355  L
C-CT-0.018900        0    -5.7332    3.16857  -15.26445  L
C-CT-0.019200        0    -5.4344    3.47794  -13.8002  L
H-H1-0.064100        0    -8.56467   4.1646   -13.88554  L
H-HC-0.025300        0    -7.08426   4.81991  -15.54136  L
H-HC-0.025300        0    -7.64882   3.30646  -16.29892  L
H-HC-0.021300        0    -5.01852   3.64871  -15.9337  L
H-HC-0.021300        0    -5.74641   2.08871  -15.41994  L
H-H1-0.039100        0    -4.75203   2.73539  -13.39222  L
H-H1-0.039100        0    -4.99516   4.47347  -13.72268  L
N-N--0.347900        0    -8.39293   1.13363  -13.21635  L
C-CT--0.240000       -1   -9.33773   0.03176  -12.92527  L
C-C-0.734100         0    -9.67048   0.05618  -11.41584  L
O-O--0.589400        0    -9.75705  -0.97825  -10.75318  L
C-CT--0.009400       0    -8.79866  -1.35396  -13.34857  L
C-CT-0.018700        0    -8.03623  -1.44691  -14.68022  L
C-CT--0.047900       0    -6.52979  -1.2594   -14.45447  L
C-CT--0.014300       0    -5.73787  -1.55218  -15.72832  L
N-N3--0.385400       0    -4.2891   -1.56567  -15.4255  L
H-H-0.274700         0    -7.73088   1.36957  -12.48437  L
H-H1-0.142600        0    -10.27345   0.2079   -13.46141  L
H-HC-0.036200        0    -9.65957  -2.02188  -13.41257  L
H-HC-0.036200        0    -8.15835  -1.75015  -12.55877  L
H-HC-0.010300        0    -8.41592  -0.71792  -15.39655  L
H-HC-0.010300        0    -8.1953   -2.44511  -15.09107  L
H-HC-0.062100        0    -6.20374  -1.94941  -13.67377  L
H-HC-0.062100        0    -6.3266   -0.24009  -14.12635  L
H-HP-0.113500        0    -5.97228  -0.78682  -16.47468  L
H-HP-0.113500        0    -6.04825  -2.52452  -16.12248  L
H-H-0.340000         0    -4.08212  -2.27795  -14.72301  L
H-H-0.340000         0    -4.02383  -0.68595  -14.98602  L
H-H-0.340000         0    -3.73068  -1.72733  -16.25004  L
N-N--0.415700        0    -9.79461   1.27173  -10.89039  L
C-CT--0.003100       -1   -10.29825   1.68213  -9.5809   L
C-C-0.597300         0    -11.24407   2.88644  -9.83952  L
N-N--0.415700        0    -10.75855   3.93412  -10.5323  L
C-CT--0.149000       -1   -11.51657   5.02517  -11.16522  L
O-O--0.567900        0    -12.42157   2.81317  -9.50448  L
C-CT--0.003600       0    -9.17752   2.02057  -8.59909  L
C-CT--0.064500       0    -8.70653   0.73423  -7.92312  L
C-C-0.695100         0    -7.53283   0.97839  -7.00115  L
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O-O--0.608600        0    -7.38412   2.01256  -6.36934  L
N-N--0.940700        0    -6.6407    0.02724  -6.89256  L
H-H-0.271900         0    -9.61873   2.02856  -11.53374  L
H-H-0.271900         0    -9.75758   3.93839  -10.68785  L
H-H1-0.085000        0    -10.91744   0.88641  -9.16011  L
H-HC-0.017100        0    -9.56077   2.69818  -7.83458  L
H-HC-0.017100        0    -8.34857   2.50529  -9.1122   L
H-HC-0.035200        0    -8.41083   0.01654  -8.68572  L
H-HC-0.035200        0    -9.52322   0.31287  -7.33807  L
H-H-0.425100         0    -5.94569   0.13891  -6.15953  L
H-H-0.425100         0    -6.79844  -0.85536  -7.34003  L
H-H1-0.097600        0    -11.61407   5.85488  -10.46219  L
H-H1-0.097600        0    -12.51527   4.67788  -11.43821  L
H-H1-0.097600        0    -10.99786   5.37399  -12.05888  L
N-N--0.415700        0    -5.33753   11.33491  -6.85441  L
C-CT--0.002400       -1   -4.3814    10.32284  -6.40876  L
C-C-0.597300         0    -2.93137   10.84444  -6.37602  L
O-O--0.567900        0    -2.66141   11.95811  -6.81736  L
C-CT--0.034300       0    -4.44533   9.10493  -7.35018  L
C-CA-0.011800        0    -5.70287   8.26219  -7.31752  L
C-CA--0.125600       0    -5.74288   7.09093  -6.53487  L
C-CA--0.170400       0    -6.80305   8.59566  -8.12857  L
C-CA--0.107200       0    -6.88228   6.26718  -6.55675  L
C-CA--0.170400       0    -7.93899   7.77152  -8.14711  L
C-CA--0.125600       0    -7.97757   6.60435  -7.36518  L
H-H-0.271900         0    -6.26618   11.0426  -7.13338  L
H-H-0.271900         0    -4.94873   12.20991  -7.19031  L
H-H1-0.097800        0    -4.64967   10.00935  -5.40383  L
H-HC-0.029500        0    -3.62442   8.43671  -7.09805  L
H-HC-0.029500        0    -4.27894   9.44454  -8.37362  L
H-HA-0.133000        0    -4.90629   6.82537  -5.90594  L
H-HA-0.143000        0    -6.78877   9.46829  -8.76315  L
H-HA-0.129700        0    -6.94023   5.38167  -5.9426   L
H-HA--0.170400       0    -8.77029   8.03842  -8.78085  L
H-HA--0.125600       0    -8.8426    5.95828  -7.37905  L
N-N--0.415700        0    -2.00127   10.01621  -5.88828  L
C-CT--0.023700       -1   -0.55127   10.11195  -6.12016  L
C-C-0.597300         0     0.07961   8.73304  -5.93551  L
O-O--0.567900        0    -0.39269   7.94393  -5.1139   L
C-CT-0.034200        0     0.0636    11.11041  -5.12154  L
C-CT-0.001800        0     1.50489   11.50913  -5.45268  L
S-S--0.273700        0     2.22308   12.63663  -4.22883  L
C-CT--0.053600       0     3.70873   13.17069  -5.11799  L
H-H-0.271900         0    -2.32447   9.13358  -5.50923  L
H-H1-0.088000        0    -0.3764    10.45911  -7.14022  L
H-HC-0.024100        0     0.04022   10.67796  -4.12089  L
H-HC-0.024100        0    -0.53154   12.02342  -5.11783  L
H-H1-0.044000        0     1.51324   11.99814  -6.42747  L
H-H1-0.044000        0     2.13259   10.62004  -5.50144  L
H-H1-0.068400        0     4.28241   13.85013  -4.48724  L
H-H1-0.068400        0     3.42066   13.68925  -6.03283  L
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H-H1-0.068400        0     4.32254   12.30701  -5.36921  L
N-N--0.415700        0     1.13678   8.44942  -6.6939   L
C-CT--0.058100       -1    1.69762   7.1083   -6.85123  L
C-C-0.597300         0     3.23248   7.16991  -6.7686   L
O-O--0.567900        0     3.93113   7.14418  -7.77854  L
C-CT--0.007400       0     1.21058   6.51616  -8.18572  L
C-CC-0.186800        0    -0.22452   6.82609  -8.51128  L
N-NB--0.543200       0    -0.64999   7.94416  -9.22526  L
C-CW--0.220700       0    -1.30291   6.06772  -8.17719  L
C-CR-0.163500        0    -1.97425   7.82003  -9.35153  L
N-NA--0.279500       0    -2.39322   6.7056   -8.72882  L
H-H-0.271900         0     1.41141   9.13648  -7.38032  L
H-H1-0.136000        0     1.34008   6.4569   -6.05534  L
H-HC-0.036700        0     1.34306   5.43606  -8.16123  L
H-HC-0.036700        0     1.80679   6.91292  -9.00815  L
H-H4-0.186200        0    -1.26902   5.13457  -7.6365   L
H-H-0.333900         0    -3.34584   6.35099  -8.77201  L
H-H5-0.143500        0    -2.60477   8.50905  -9.89912  L
N-N--0.415700        0     3.77178   7.33019  -5.56012  L
C-CT--0.059700       -1    5.18459   7.67433  -5.35039  L
C-C-0.597300         0     6.13851   6.51057  -5.68495  L
O-O--0.567900        0     5.84529   5.36267  -5.33712  L
C-CT-0.130300        0     5.43091   8.22858  -3.92331  L
C-CT--0.043000       0     5.14439   7.22183  -2.78471  L
C-CT--0.320400       0     4.61396   9.51982  -3.73751  L
C-CT--0.066000       0     5.49614   7.73637  -1.38304  L
H-H-0.271900         0     3.14568   7.29014  -4.76232  L
H-H1-0.086900        0     5.3809    8.49236  -6.0357   L
H-HC-0.018700        0     6.48614   8.50135  -3.8642   L
H-HC-0.023600        0     5.71665   6.31525  -2.95856  L
H-HC-0.023600        0     4.09441   6.95171  -2.78412  L
H-HC-0.088200        0     3.54993   9.29441  -3.65379  L
H-HC-0.088200        0     4.77459   10.18907  -4.58115  L
H-HC-0.088200        0     4.93268   10.03758  -2.83346  L
H-HC-0.018600        0     4.79207   8.51138  -1.0815   L
H-HC-0.018600        0     6.50762   8.14181  -1.37282  L
H-HC-0.018600        0     5.42934   6.91478  -0.66959  L
N-N--0.254800        0     7.28011   6.77006  -6.35061  L
C-CT--0.026600       -1    8.11835   5.72069  -6.924    L
C-C-0.589600         0     8.59168   4.58781  -6.02209  L
O-O--0.574800        0     8.7575    4.77801  -4.81578  L
C-CT--0.007000       0     9.31631   6.44227  -7.54151  L
C-CT-0.018900        0     8.74103   7.78939  -7.94879  L
C-CT-0.019200        0     7.72957   8.07247  -6.84219  L
H-H1-0.064100        0     7.55631   5.28453  -7.74018  L
H-HC-0.025300        0     9.69656   5.9015   -8.40765  L
H-HC-0.025300        0     10.09704   6.58998  -6.79337  L
H-HC-0.021300        0     8.2207    7.68962  -8.90313  L
H-HC-0.021300        0     9.50916   8.56098  -8.00729  L
H-H1-0.039100        0     8.20851   8.62254  -6.0313   L
H-H1-0.039100        0     6.91853   8.65856  -7.27242  L
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N-N--0.415700        0     8.85765   3.42562  -6.62216  L
C-CT--0.051800       -1    9.2724    2.20327  -5.92964  L
C-C-0.597300         0     10.50454   2.39771  -5.01995  L
O-O--0.567900        0     11.53962   2.90365  -5.4558   L
C-CT--0.110200       0     9.50235   1.06631  -6.93394  L
C-CT-0.353100        0     8.26819   0.62416  -7.74153  L
C-CT--0.412100       0     8.63465  -0.56896  -8.62414  L
C-CT--0.412100       0     7.09024   0.23159  -6.852    L
H-H-0.271900         0     8.69945   3.39137  -7.63093  L
H-H1-0.092200        0     8.45261   1.91     -5.2776   L
H-HC-0.045700        0     9.86764   0.20439  -6.37577  L
H-HC-0.045700        0     10.28068   1.38002  -7.62977  L
H-HC--0.036100       0     7.93791   1.42594  -8.38874  L
H-HC-0.100000        0     9.01815  -1.38474  -8.0169   L
H-HC-0.100000        0     9.39459  -0.25587  -9.34148  L
H-HC-0.100000        0     7.75927  -0.89973  -9.18237  L
H-HC-0.100000        0     7.40318  -0.47424  -6.08556  L
H-HC-0.100000        0     6.31723  -0.21079  -7.47658  L
H-HC-0.100000        0     6.6744    1.11911  -6.37723  L
N-N--0.415700        0     10.40337   1.93449  -3.76567  L
C-CT--0.059700       -1    11.55786   1.50869  -2.95043  L
C-C-0.597300         0     11.90488   0.09266  -3.42091  L
O-O--0.567900        0     11.05752  -0.8083   -3.38791  L
C-CT-0.130300        0     11.23171   1.55985  -1.4416   L
C-CT--0.043000       0     10.75825   2.95569  -0.96762  L
C-CT--0.320400       0     12.44306   1.10108  -0.6099   L
C-CT--0.066000       0     11.65712   4.13721  -1.35708  L
H-H-0.271900         0     9.4923    1.57398  -3.50296  L
H-H1-0.086900        0     12.40471   2.16571  -3.15228  L
H-HC-0.018700        0     10.41746   0.86028  -1.24409  L
H-HC-0.023600        0     10.67155   2.95048   0.11832  L
H-HC-0.023600        0     9.76156   3.13865  -1.36836  L
H-HC-0.088200        0     12.66997   0.05616  -0.8233   L
H-HC-0.088200        0     12.22152   1.18918   0.45377  L
H-HC-0.088200        0     13.31886   1.70653  -0.84621  L
H-HC-0.018600        0     11.28893   5.0432   -0.87712  L
H-HC-0.018600        0     11.63324   4.28537  -2.43633  L
H-HC-0.018600        0     12.68203   3.96412  -1.03052  L
N-N--0.415700        0     13.12637  -0.07923  -3.91843  L
C-CT--0.051800       -1    13.56196  -1.21744  -4.72115  L
C-C-0.597300         0     14.6108  -2.07049  -4.02343  L
O-O--0.567900        0     15.38182  -1.60109  -3.18973  L
C-CT--0.110200       0     14.13281  -0.72185  -6.07228  L
C-CT-0.353100        0     13.17376   0.03627  -7.00546  L
C-CT--0.412100       0     13.96896   0.74324  -8.10393  L
C-CT--0.412100       0     12.20092  -0.91777  -7.69156  L
H-H-0.271900         0     13.72524   0.74036  -3.92683  L
H-H1-0.092200        0     12.69916  -1.84935  -4.92123  L
H-HC-0.045700        0     14.53445  -1.57456  -6.62121  L
H-HC-0.045700        0     14.97091  -0.0661   -5.86172  L
H-HC--0.036100       0     12.61759   0.78159  -6.44466  L
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H-HC-0.100000        0     14.51963   0.01864  -8.70314  L
H-HC-0.100000        0     14.67061   1.44747  -7.66008  L
H-HC-0.100000        0     13.28652   1.29774  -8.75042  L
H-HC-0.100000        0     11.59068  -0.36287  -8.40286  L
H-HC-0.100000        0     11.55502  -1.37559  -6.94723  L
H-HC-0.100000        0     12.75087  -1.67939  -8.2367   L
N-N--0.415700        0     14.68709  -3.31965  -4.45522  L
C-CT--0.025200       -1    15.80039  -4.20445  -4.19262  L
C-C-0.597300         0     15.82075  -5.43077  -5.11367  L
N-N--0.415700        0     16.58964  -6.4531   -4.72714  L
C-CT--0.149000       0     16.82295  -7.67084  -5.50127  L
O-O--0.567900        0     15.15862  -5.46018  -6.15826  L
H-H-0.271900         0     13.99118  -3.62475  -5.12799  L
H-H-0.271900         0     17.05279  -6.36577  -3.8236   L
H-H1-0.069800        0     15.76108  -4.54749  -3.16067  L
H-H1-0.069800        0     16.73467  -3.66003  -4.3333   L
H-H1-0.097600        0     17.47847  -7.44873  -6.34589  L
H-H1-0.097600        0     15.88004  -8.06626  -5.88042  L
H-H1-0.097600        0     17.30294  -8.42274  -4.87177  L
N-N--0.415700        0     13.78754  -4.16695  -8.53502  L
C-CT--0.038900       -1    12.40035  -4.64819  -8.39778  L
C-C-0.597300         0     11.77059  -4.20549  -7.06111  L
O-O--0.567900        0     12.53208  -3.91229  -6.14202  L
C-CT-0.365400        0     12.3595  -6.18797  -8.49567  L
O-OH--0.676100       0     13.12941  -6.83206  -7.49845  L
C-CT--0.243800       0     12.85928  -6.70045  -9.84519  L
H-H-0.271900         0     14.38599  -4.19031  -7.71247  L
H-H-0.271900         0     14.14758  -3.84969  -9.42594  L
H-H1-0.100700        0     11.80083  -4.23194  -9.20685  L
H-H1-0.004300        0     11.33291  -6.51924  -8.38043  L
H-HC-0.064200        0     12.71739  -7.77992  -9.89854  L
H-HC-0.064200        0     13.91895  -6.47786  -9.97267  L
H-HC-0.064200        0     12.29102  -6.23445  -10.65043  L
H-HO-0.410200        0     13.83757  -6.22422  -7.21443  L
N-N--0.254800        0     10.43189  -4.12393  -6.89634  L
C-CT--0.026600       -1    9.81166  -3.62316  -5.65834  L
C-C-0.589600         0     10.19116  -4.4695   -4.44299  L
O-O--0.574800        0     10.04723  -5.6932   -4.44239  L
C-CT--0.007000       0     8.30252  -3.61015  -5.91427  L
C-CT-0.018900        0     8.11861  -4.63301  -7.03109  L
C-CT-0.019200        0     9.3941   -4.47138  -7.85777  L
H-H1-0.064100        0     10.13796  -2.59766  -5.48117  L
H-HC-0.025300        0     8.0025   -2.62991  -6.27679  L
H-HC-0.025300        0     7.73231  -3.86706  -5.02215  L
H-HC-0.021300        0     7.2224   -4.43667  -7.62049  L
H-HC-0.021300        0     8.08711  -5.63458  -6.60065  L
H-H1-0.039100        0     9.60592  -5.39711  -8.38708  L
H-H1-0.039100        0     9.27039  -3.65623  -8.57155  L
N-N--0.415700        0     10.71542  -3.80506  -3.41563  L
C-CT--0.051800       -1    11.19534  -4.4353   -2.19218  L
C-C-0.597300         0     10.0466  -5.0111   -1.36202  L
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 O-O--0.567900        0     9.0244   -4.34959  -1.17493  L
 C-CT--0.110200       0     11.95197  -3.36249  -1.38531  L
 C-CT-0.353100        0     12.88447  -3.94253  -0.30723  L
 C-CT--0.412100       0     14.20726  -4.38887  -0.92806  L
 C-CT--0.412100       0     13.18218  -2.87431   0.74008  L
 H-H-0.271900         0     10.78933  -2.79668  -3.48586  L
 H-H1-0.092200        0     11.88177  -5.23649  -2.46357  L
 H-HC-0.045700        0     11.21483  -2.70787  -0.9163   L
 H-HC-0.045700        0     12.54801  -2.74577  -2.05879  L
 H-HC--0.036100       0     12.41178  -4.78844   0.19082  L
 H-HC-0.100000        0     14.68654  -3.54227  -1.418    L
 H-HC-0.100000        0     14.03062  -5.18298  -1.65218  L
 H-HC-0.100000        0     14.88546  -4.76     -0.16384  L
 H-HC-0.100000        0     13.6292   -2.00112   0.26667  L
 H-HC-0.100000        0     13.86973  -3.26408   1.48935  L
 H-HC-0.100000        0     12.25121  -2.58916   1.22739  L
 N-N--0.415700        0     10.23938  -6.22426  -0.84389  L
 C-CT--0.024900       -1    9.28831   -6.89795   0.03567  L
 C-C-0.597300         0     9.98225   -7.88609   0.98289  L
 O-O--0.567900        0     11.1973   -7.86422   1.19345  L
 C-CT-0.211700        0     8.18218   -7.51549  -0.83772  L
 O-OH--0.654600       0     7.09158   -7.95661  -0.04538  L
 H-H-0.271900         0     11.10427  -6.71262  -1.05426  L
 H-H1-0.084300        0     8.81811   -6.13953   0.66394  L
 H-H1-0.035200        0     8.59166   -8.34993  -1.40891  L
 H-H1-0.035200        0     7.8157    -6.76276  -1.53781  L
 H-HO-0.427500        0     6.29131   -7.42848  -0.28625  L
 N-N--0.347900        0     9.17162   -8.73063   1.60816  L
 C-CT--0.240000       -1    9.47891   -9.77849   2.57946  L
 C-C-0.734100         0     10.41043  -10.85196   2.00302  L
 O-O--0.589400        0     11.36459  -11.24146   2.66916  L
 C-CT--0.009400       0     8.11189   -10.33114   3.07029  L
 C-CT-0.018700        0     7.20564   -9.26432   3.7532   L    H-HC
1455  0.        0.
 C-CT--0.047900       0     5.68044   -9.44145   3.58111  H
 C-CT--0.014300       0     5.1709    -9.08682   2.1875   H
 N-N3--0.385400       0     3.6591    -9.05055   2.15528  H
 H-H-0.274700         0     8.20561   -8.62997   1.31591  L
 H-H1-0.142600        0     10.00759   -9.33789   3.42677  L
 H-HC-0.036200        0     8.28841   -11.1419   3.77914  L
 H-HC-0.036200        0     7.57973   -10.75744   2.22075  L
 H-HC-0.010300        0     7.45315   -8.2626    3.40236  L
 H-HC-0.010300        0     7.431     -9.27893   4.82059  L
 H-HC-0.062100        0     5.2002    -8.78097   4.31162  H
 H-HC-0.062100        0     5.41847   -10.47278   3.83308  H
 H-HP-0.113500        0     5.47834   -9.8182    1.43857  H
 H-HP-0.113500        0     5.49146   -8.09934   1.85594  H
 H-H-0.340000         0     3.2405    -9.75155   2.78674  H
 H-H-0.340000         0     3.29986   -9.29404   1.22072  H
 H-H-0.340000         0     3.17343   -8.10984   2.40146  H
 N-N--0.347900        0     10.19344   -11.21363   0.73094  L
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C-CT--0.263700       -1    11.12319  -11.81198  -0.25536  L
C-C-0.734100         0     12.61411  -11.53534  -0.01086  L
O-O--0.589400        0     13.43811  -12.40482  -0.26559  L
C-CT--0.000700       0     10.66081  -11.30575  -1.63415  L
C-CT-0.039000        0     11.61686  -11.55299  -2.81241  L
C-CT-0.048600        0     10.95855  -10.99688  -4.08006  L
N-N2--0.529500       0     11.92629  -10.75753  -5.16765  L
C-CA-0.807600        0     11.83838  -9.80646  -6.08391  L
N-N2--0.862700       0     10.85092  -8.96464  -6.13518  L
N-N2--0.862700       0     12.7714  -9.65503  -6.97623  L
H-H-0.274700         0     9.2981   -10.89904   0.36541  L
H-H1-0.156000        0     11.01903  -12.89792  -0.22963  L
H-HC-0.032700        0     10.50032  -10.22745  -1.56251  L
H-HC-0.032700        0     9.69851  -11.76842  -1.86186  L
H-HC-0.028500        0     11.81405  -12.61957  -2.92785  L
H-HC-0.028500        0     12.55424  -11.02307  -2.63774  L
H-H1-0.068700        0     10.4876  -10.05416  -3.81258  L
H-H1-0.068700        0     10.17853  -11.6836  -4.41554  L
H-H-0.345600         0     12.72635  -11.36383  -5.20885  L
H-H-0.447800         0     10.64734  -8.42869  -6.97179  L
H-H-0.447800         0     10.13692  -8.96093  -5.40842  L
H-H-0.447800         0     12.76495  -8.77313  -7.47837  L
H-H-0.447800         0     13.54818  -10.28246  -7.0433   L
N-N--0.415700        0     12.96597  -10.32099   0.40738  L
C-CT--0.058100       -1    14.33953  -9.81743   0.4941   L
C-C-0.597300         0     14.94943  -9.81441   1.90422  L
N-N--0.415700        0     14.23468  -10.32816   2.9134   L
C-CT--0.149000       0     14.69188  -10.45026   4.29537  L
O-O--0.567900        0     16.07591  -9.33788   2.06254  L
C-CT--0.007400       0     14.31067  -8.39064  -0.08849  L
C-CC-0.186800        0     13.77246  -8.23578  -1.49458  L
N-NB--0.543200       0     12.42868  -8.06405  -1.83124  L
C-CW--0.220700       0     14.52613  -8.07324  -2.61938  L
C-CR-0.163500        0     12.39986  -7.81146  -3.14777  L
N-NA--0.279500       0     13.64644  -7.80336  -3.64924  L
H-H-0.271900         0     12.21987  -9.65169   0.54094  L
H-H-0.271900         0     13.31764  -10.70011   2.68488  L
H-H1-0.136000        0     14.99529  -10.42892  -0.12815  L
H-HC-0.036700        0     15.30958  -7.96225  -0.06218  L
H-HC-0.036700        0     13.67907  -7.78824   0.55616  L
H-H4-0.186200        0     15.60723  -8.09014  -2.65601  L
H-H-0.333900         0     13.87962  -7.56571  -4.60509  L
H-H5-0.143500        0     11.50151  -7.60685  -3.71602  L
H-H1-0.097600        0     15.40841  -9.66159   4.52986  L
H-H1-0.097600        0     15.17784  -11.41797   4.43339  L
H-H1-0.097600        0     13.8391  -10.38102   4.97216  L
N-N--0.415700        0     14.61706  -6.77646   5.50413  L
C-CT--0.038900       -1    13.92842  -5.60318   4.93485  L
C-C-0.597300         0     12.71941  -5.11074   5.74676  L
O-O--0.567900        0     12.12347  -4.07998   5.41695  L
C-CT-0.365400        0     13.46959  -5.8882    3.49635  L
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O-OH--0.676100       0     12.77779  -7.11927   3.44641  L
C-CT--0.243800       0     14.67892  -5.96132   2.57161  L
H-H-0.271900         0     14.42135  -7.6672    5.05828  L
H-H-0.271900         0     15.40751  -6.66813   6.12704  L
H-H1-0.100700        0     14.62736  -4.76781   4.90552  L
H-H1-0.004300        0     12.81619  -5.08685   3.14916  L
H-HC-0.064200        0     14.3328   -6.02128   1.54778  L
H-HC-0.064200        0     15.28743  -6.83552   2.80317  L
H-HC-0.064200        0     15.28505  -5.06132   2.6753   L
H-HO-0.410200        0     12.39109  -7.23923   2.56304  L
N-N--0.415700        0     12.37121  -5.8107    6.82996  L
C-CT--0.024900       -1    11.47211  -5.32874   7.88564  L
C-C-0.597300         0     11.99621  -4.04085   8.51876  L
O-O--0.567900        0     13.2031   -3.90158   8.70125  L
C-CT-0.211700        0     11.32531  -6.39983   8.96904  L
O-OH--0.654600       0     12.60002  -6.82921   9.4097   L
H-H-0.271900         0     12.92362  -6.62731   7.04847  L
H-H1-0.084300        0     10.49741  -5.14356   7.44687  L
H-H1-0.035200        0     10.7856   -7.25446   8.55884  L
H-H1-0.035200        0     10.75835  -5.99776   9.81042  L
H-HO-0.427500        0     13.11874  -6.05199   9.66439  L
N-N--0.415700        0     11.0941   -3.13383   8.8986   L
C-CT--0.087500       -1    11.43636  -1.90708   9.64743  L
C-C-0.597300         0     12.16006  -2.21671   10.96646  L
N-N--0.415700        0     11.68617  -3.22735   11.71347  L
O-O--0.567900        0     13.11265  -1.52316   11.31172  L
C-CT-0.298500        0     10.18292  -1.06195   9.92722  L
C-CT--0.319200       0     10.47063   0.2128    10.73367  L
C-CT--0.319200       0     9.54085   -0.61361   8.61521  L
H-H-0.271900         0     10.11956  -3.35016   8.7203   L
H-H-0.096900         0     10.89163  -3.74401   11.36904  L
H-H1-0.096900        0     12.12679  -1.31432   9.04711  L
H-HC--0.029700       0     9.45825   -1.66426   10.47729  L
H-HC-0.079100        0     9.56386    0.80786   10.83738  L
H-HC-0.079100        0     11.23961   0.80501   10.23613  L
H-HC-0.079100        0     10.82014  -0.04529   11.73394  L
H-HC-0.079100        0     9.25791   -1.473     8.0106   L
H-HC-0.079100        0     10.23156   0.01408   8.05252  L
H-HC-0.079100        0     8.64752   -0.04904   8.85941  L
N-N--0.415700        0     14.06303   7.18241   5.65651  L
C-CT--0.051800       -1    13.44838   6.52198   4.49701  L
C-C-0.597300         0     12.89605   7.49829   3.43977  L
O-O--0.567900        0     12.6435    7.08122   2.31564  L
C-CT--0.110200       0     12.33477   5.56408   4.96681  L
C-CT-0.353100        0     12.75999   4.45862   5.95296  L
C-CT--0.412100       0     11.54116   3.61218   6.32107  L
C-CT--0.412100       0     13.8305    3.54096   5.36033  L
H-H-0.271900         0     13.56251   7.20439   6.53706  L
H-H-0.271900         0     15.06048   7.36208   5.65375  L
H-H1-0.092200        0     14.21304   5.93172   3.99063  L
H-HC-0.045700        0     11.91787   5.08164   4.08268  L
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H-HC-0.045700        0     11.54028   6.1528    5.42672  L
H-HC--0.036100       0     13.14806   4.91217   6.86496  L
H-HC-0.100000        0     11.82849   2.84449   7.03979  L
H-HC-0.100000        0     11.13286   3.13776   5.42978  L
H-HC-0.100000        0     10.77497   4.24213   6.77281  L
H-HC-0.100000        0     14.0183   2.70782   6.03869  L
H-HC-0.100000        0     14.7633   4.08825   5.23294  L
H-HC-0.100000        0     13.50217   3.15456   4.39581  L
N-N--0.415700        0     12.72409   8.78077   3.77518  L
C-CT-0.033700        0     12.36722   9.83968   2.82329  L
C-C-0.597300         0     13.52052   10.16389   1.84695  L
N-N--0.415700        0     14.73242   10.38977   2.37449  L
C-CT--0.149000       -1    15.9548   10.66249   1.61699  L
O-O--0.567900        0     13.31668   10.20285   0.6347   L
C-CT--0.182500       0     11.92255   11.07736   3.61354  L
H-H-0.271900         0     12.90312   9.03792   4.73203  L
H-H-0.271900         0     14.79098   10.38768   3.37984  L
H-H1-0.082300        0     11.5218   9.50062   2.22037  L
H-HC-0.060300        0     12.73448   11.44687   4.24114  L
H-HC-0.060300        0     11.06441   10.83004   4.24029  L
H-HC-0.060300        0     11.62705   11.8651   2.91806  L
H-H1-0.097600        0     15.71325   11.03777   0.61983  L
H-H1-0.097600        0     16.54551   9.75053   1.527    L
H-H1-0.097600        0     16.54953   11.41958   2.13204  L
N-N--0.415700        0     14.85199   7.20604   0.55915  L
C-CT--0.051800       -1    15.1246   7.89241  -0.70006  L
C-C-0.597300         0     13.85588   8.06151  -1.55138  L
O-O--0.567900        0     12.81982   7.45614  -1.2766   L
C-CT--0.110200       0     16.19629   7.09208  -1.47563  L
C-CT-0.353100        0     17.59412   7.05243  -0.83074  L
C-CT--0.412100       0     18.46359   6.02722  -1.55732  L
C-CT--0.412100       0     18.29598   8.40912  -0.91097  L
H-H-0.271900         0     13.88236   7.19514   0.87684  L
H-H-0.271900         0     15.4823   6.48546   0.87727  L
H-H1-0.092200        0     15.49902   8.89203  -0.48648  L
H-HC-0.045700        0     16.30471   7.50735  -2.47784  L
H-HC-0.045700        0     15.83624   6.0676   -1.58615  L
H-HC--0.036100       0     17.50969   6.75337   0.21424  L
H-HC-0.100000        0     19.45003   5.98315  -1.09486  L
H-HC-0.100000        0     18.57661   6.30026  -2.60696  L
H-HC-0.100000        0     18.0094   5.03751  -1.49555  L
H-HC-0.100000        0     18.40979   8.71439  -1.95182  L
H-HC-0.100000        0     19.28578   8.3355   -0.45868  L
H-HC-0.100000        0     17.7305   9.16682  -0.37483  L
N-N--0.415700        0     13.95946   8.84912  -2.62263  L
C-CT--0.025200       -1    12.95298   8.98315  -3.67895  L
C-C-0.597300         0     12.92718   10.397   -4.26791  L
N-N--0.415700        0     12.67237   10.5142  -5.57574  L
C-CT--0.149000       0     12.61008   11.79098  -6.28642  L
O-O--0.567900        0     13.12312   11.36631  -3.53622  L
H-H-0.271900         0     14.81011   9.38139  -2.72854  L
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H-H-0.271900          0     12.53469   9.67103  -6.111    L
H-H1-0.069800         0     11.96159   8.76925  -3.28396  L
H-H1-0.069800         0     13.16874   8.26772  -4.47171  L
H-H1-0.097600         0     11.82853   12.42003  -5.85502  L
H-H1-0.097600         0     12.39444   11.62776  -7.34382  L
H-H1-0.097600         0     13.56461   12.3141  -6.19522  L
N-N--0.415700         0     12.23831   5.47834  -9.54299  L
C-CT--0.025200        -1    12.35555   4.65242  -8.34445  L
C-C-0.597300          0     13.78173   4.62758  -7.78721  L
O-O--0.567900         0     14.69471   5.1943   -8.38567  L
H-H-0.271900          0     11.43937   5.34449  -10.16255  L
H-H-0.271900          0     13.09396   5.87715  -9.91068  L
H-H1-0.069800         0     12.06484   3.62938  -8.58148  L
H-H1-0.069800         0     11.69105   5.02588  -7.56897  L
N-N--0.415700         0     13.97738   4.01297  -6.61707  L
C-CT--0.087500        -1    15.23832   4.07248  -5.85129  L
C-C-0.597300          0     15.52462   2.78534  -5.08085  L
O-O--0.567900         0     14.6369   2.20226  -4.46571  L
C-CT-0.298500         0     15.23264   5.24909  -4.85055  L
C-CT--0.319200        0     15.36248   6.60574  -5.55232  L
C-CT--0.319200        0     13.98013   5.28133  -3.96371  L
H-H-0.271900          0     13.17852   3.55436  -6.18272  L
H-H1-0.096900         0     16.06416   4.22624  -6.54669  L
H-HC--0.029700        0     16.10291   5.1441   -4.20112  L
H-HC-0.079100         0     16.22756   6.59408  -6.21661  L
H-HC-0.079100         0     15.50156   7.3944   -4.81513  L
H-HC-0.079100         0     14.47136   6.81704  -6.14234  L
H-HC-0.079100         0     14.05043   6.1036   -3.26489  L
H-HC-0.079100         0     13.90144   4.36035  -3.38969  L
H-HC-0.079100         0     13.07855   5.40578  -4.56335  L
N-N--0.415700         0     16.77968   2.338    -5.09015  L
C-CT--0.059700        -1    17.22243   1.12664  -4.38477  L
C-C-0.597300          0     17.42443   1.39509  -2.89536  L
O-O--0.567900         0     17.9995   2.40653  -2.49161  L
C-CT-0.130300         0     18.49324   0.54653  -5.05684  L
C-CT--0.043000        0     18.17212   0.13046  -6.51569  L
C-CT--0.320400        0     19.03706  -0.66757  -4.27625  L
C-CT--0.066000        0     19.39958  -0.25552  -7.35156  L
H-H-0.271900          0     17.47443   2.8832   -5.57675  L
H-H1-0.086900         0     16.44529   0.37185  -4.46168  L
H-HC-0.018700         0     19.26337   1.32032  -5.07076  L
H-HC-0.023600         0     17.6928   0.95931  -7.03616  L
H-HC-0.023600         0     17.47148  -0.70591  -6.50955  L
H-HC-0.088200         0     19.9155  -1.08003  -4.77034  L
H-HC-0.088200         0     18.27375  -1.44259  -4.19613  L
H-HC-0.088200         0     19.35639  -0.37116  -3.27707  L
H-HC-0.018600         0     20.14615   0.53811  -7.30593  L
H-HC-0.018600         0     19.09662  -0.39556  -8.38964  L
H-HC-0.018600         0     19.83347  -1.18832  -6.99332  L
N-N--0.415700         0     16.96258   0.45682  -2.07341  L
C-CT--0.002400        -1    17.24462   0.41721  -0.65165  L
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C-C-0.597300          0     18.70649   0.00045  -0.3692   L
N-N--0.415700         0     19.61521   0.98659  -0.32243  L
C-CT--0.149000        -1    21.04044   0.82591  -0.01093  L
O-O--0.567900         0     19.00586  -1.18087  -0.20565  L
C-CT--0.034300        0     16.21373  -0.47727   0.05182  L
C-CA-0.011800         0     16.31477  -0.43235   1.56503  L
C-CA--0.125600        0     15.95005   0.73715   2.26094  L
C-CA--0.125600        0     16.81005  -1.54093   2.27679  L
C-CA--0.170400        0     16.08618   0.79873   3.66007  L
C-CA--0.170400        0     16.93565  -1.4831    3.67636  L
C-CA--0.107200        0     16.57603  -0.31317   4.36789  L
H-H-0.271900          0     16.48682  -0.34261  -2.47903  L
H-H-0.271900          0     19.28113   1.90021  -0.59867  L
H-H1-0.097800         0     17.11823   1.42502  -0.256    L
H-HC-0.029500         0     16.32835  -1.5054   -0.29629  L
H-HC-0.029500         0     15.21418  -0.14584  -0.23047  L
H-HA-0.133000         0     15.57527   1.59304   1.71932  L
H-HA-0.133000         0     17.12113  -2.42938   1.74442  L
H-HA-0.143000         0     15.82091   1.69892   4.19426  L
H-HA-0.143000         0     17.33255  -2.33036   4.21807  L
H-HA-0.129700         0     16.68914  -0.26755   5.44264  L
H-H1-0.097600         0     21.49149   0.11655  -0.70779  L
H-H1-0.097600         0     21.15517   0.4374    1.00283  L
H-H1-0.097600         0     21.55598   1.78394  -0.0914   L
C-CT-0.055800         0    -6.54154  -9.61187  -6.40716  L
C-CT-0.106500         0    -6.07213  -10.7831  -5.54175  L
O-OS--0.354800        0    -4.90439  -11.33912  -6.13643  L
C-CT-0.202200         0    -5.69443  -10.45779  -4.08756  L
O-OS--0.495400        0    -6.75475  -10.45693  -3.14264  L
C-CT-0.067000         0    -4.80527  -11.67599  -3.80364  L
O-OH--0.613900        0    -5.56758  -12.86893  -3.61127  L
C-CT-0.006600         0    -4.03729  -11.8359  -5.11691  L
N-N*--0.048400        0    -2.7251   -11.11476  -5.11712  L
C-C-0.753800          0    -1.58726  -11.7845  -4.65531  L
O-O--0.625800         0    -1.64049  -12.91694  -4.17478  L
N-NC--0.758400        0    -0.36199  -11.1506  -4.74374  L
C-CA--0.521500        0    -0.23618  -9.95705  -5.26969  L
N-N2--0.953800        0     0.98039  -9.54246  -5.49995  L
C-CM--0.521500        0    -1.3668   -9.25486  -5.74767  L
C-CM-0.005300         0    -2.58301  -9.85332  -5.64963  L
H-HC-0.067900         0    -7.42022  -9.13967  -5.98009  L
H-HC-0.067900         0    -5.74288  -8.88165  -6.50121  L
H-H1-0.117400         0    -6.84709  -11.54948  -5.5241   L
H-H1-0.061500         0    -5.09019  -9.55072  -4.03178  L
H-H1-0.097200         0    -4.13494  -11.50131  -2.96246  L
H-HO-0.418600         0    -5.73648  -13.00683  -2.6499   L
H-H2-0.202900         0    -3.84392  -12.90259  -5.26928  L
H-H-0.423900          0     1.78747  -10.1359  -5.3081   L
H-H-0.423900          0     1.20226  -8.70368  -6.04874  L
H-HA-0.192800         0    -1.35896  -8.2771   -6.2124   L
H-H4-0.195800         0    -3.44917  -9.33674  -6.03415  L
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 P-P-1.166200         0    -7.51266  -9.14522  -2.66445  L
 O-O2--0.776000       0    -8.23447  -9.55433  -1.44425  L
 O-O2--0.776000       0    -8.32369  -8.65137  -3.79113  L
 O-OS--0.498900       0    -6.38607  -8.0518   -2.31356  L
 C-CT-0.055800        0    -5.47281  -8.15313  -1.22281  L    H-H1
1732  0.        0.
 C-CT-0.106500        0    -4.30662  -7.12585  -1.28477  H
 O-OS--0.354800       0    -3.41451  -7.50733  -2.34516  H
 C-CT-0.202200        0    -4.63636  -5.66181  -1.59269  H
 O-OH--0.654100       0    -5.13465  -4.90678  -0.53098  H
 C-CT-0.067000        0    -3.29534  -5.12763  -2.14431  H
 O-OH--0.613900       0    -2.3413   -4.81507  -1.13826  H
 C-CT-0.039400        0    -2.86347  -6.37229  -2.97048  H
 N-N*--0.025100       0    -3.38119  -6.33201  -4.34452  H
 C-CK-0.200600        0    -4.66714  -6.67205  -4.70354  H
 N-NB--0.607300       0    -4.95546  -6.47666  -5.95927  H
 C-CB-0.051500        0    -3.78732  -5.97318  -6.47711  H
 C-CA-0.700900        0    -3.47738  -5.45972  -7.74828  H
 N-N2--0.901900       0    -4.42639  -5.32985  -8.71078  H
 N-NC--0.761500       0    -2.21443  -5.0931   -8.00173  H
 C-CQ-0.587500        0    -1.31775  -5.20068  -7.00937  H
 N-NC--0.699700       0    -1.51179  -5.54108  -5.73489  H
 C-CB-0.305300        0    -2.78135  -5.90384  -5.51259  H
 H-H1-0.067900        0    -5.0475   -9.15739  -1.18917  L
 H-H1-0.067900        0    -6.02455  -7.98582  -0.29957  L
 H-H1-0.117400        0    -3.77672  -7.15459  -0.32433  H
 H-H1-0.061500        0    -5.30915  -5.62283  -2.45052  H
 H-HO-0.437600        0    -6.03726  -5.2111   -0.30855  H
 H-H1-0.097200        0    -3.42992  -4.2668   -2.80955  H
 H-HO-0.418600        0    -0.71644  -5.43752  -1.29603  H
 H-H2-0.200700        0    -1.77566  -6.442    -3.01576  H
 H-H5-0.155300        0    -5.34307  -7.08147  -3.98084  H
 H-H-0.411500         0    -4.21971  -4.69752  -9.47523  H
 H-H-0.411500         0    -5.39457  -5.30787  -8.39913  H
 H-H5-0.047300        0    -0.29814  -4.9465   -7.27462  H
 C-CQ-0.587500        0     6.59092   1.85393  -3.00304  L
 P-P-1.166200         0     0.32097  -3.10248   0.83016  H
 N-N3-0.001700        0    -3.75849  -2.95587   0.72226  H
 C-CT-0.058800        0    -3.19686  -2.5599   -0.57413  H
 C-CT-0.090900        0    -3.01264  -1.0344   -0.60382  H
 C-CT--0.023600       0    -2.78524  -0.36777  -1.97435  H
 C-C-0.808700         0    -3.23775   1.09607  -1.94059  H
 O-O2--0.818900       0    -2.5385    1.93221  -1.32591  H
 O-O2--0.818900       0    -4.35058   1.37092  -2.52737  H
 C-C-0.562100         0    -1.93198  -3.34221  -0.98716  H
 O-O--0.588900        0    -1.1965   -2.91753  -1.89945  H
 O-OS--0.421000       0    -1.1251   -3.57072   0.39383  H
 O-O2--0.776000       0     1.38226  -4.00153   0.10926  H
 O-O2--0.776000       0     0.49632  -3.14916   2.33001  H
 O-OS--0.498900       0     0.63847  -1.61988   0.33048  H
 C-CT-0.055800        0     0.77672  -0.59295   1.32871  H
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 C-CT-0.106500        0     1.14436   0.75588   0.68823  L    H-H1
1776  0.        0.
 O-OS--0.354800       0     2.54178   0.92068   0.43788  L
 C-CT-0.039400        0     2.77624   1.05419  -0.96636  L
 N-N*--0.025100       0     3.918     0.18065  -1.33825  L
 C-CB-0.305300        0     5.07646   0.56697  -1.98256  L
 N-NC--0.699700       0     5.35241   1.78143  -2.52886  L
 N-NC--0.761500       0     7.54004   0.92318  -2.98619  L
 C-CA-0.700900        0     7.22292  -0.26194  -2.45967  L
 N-N2--0.901900       0     8.21834  -1.13448  -2.46641  L
 C-CB-0.051500        0     5.93237  -0.50161  -1.91683  L
 N-NB--0.607300       0     5.30952  -1.59266  -1.29702  L
 C-CK-0.200600        0     4.12249  -1.13157  -0.98687  L
 C-CT-0.067000        0     1.4683    0.70258  -1.67589  L
 O-OH--0.613900       0     1.29728   1.41972  -2.89012  L
 C-CT-0.202200        0     0.40484   1.01987  -0.61567  L
 O-OH--0.654100       0    -0.06527   2.35721  -0.58452  L
 H-H5-0.047300        0     6.86335   2.79867  -3.45203  L
 H-H-0.239100         0    -3.13946  -2.63845   1.47334  H
 H-H-0.239100         0    -3.83083  -3.9674    0.80883  H
 H-H-0.239100         0    -5.31343  -2.38881   0.7517   H
 H-HP-0.120200        0    -3.95665  -2.8159   -1.32414  H
 H-HC--0.023200       0    -2.18039  -0.74924   0.04672  H
 H-HC--0.023200       0    -3.94224  -0.64683  -0.17645  H
 H-HC--0.031500       0    -3.33092  -0.89802  -2.75329  H
 H-HC--0.031500       0    -1.72956  -0.41362  -2.23762  H
 H-H1-0.067900        0     1.54377  -0.85934   2.05586  H
 H-H1-0.067900        0    -0.17647  -0.47085   1.85539  H
 H-H1-0.117400        0     0.84294   1.52186   1.39967  L
 H-H2-0.200700        0     3.01953   2.08947  -1.2179   L
 H-H-0.411500         0     8.07133  -2.06739  -2.10391  L
 H-H-0.411500         0     9.10183  -0.85699  -2.87148  L
 H-H5-0.155300        0     3.36473  -1.71643  -0.47627  L
 H-H1-0.097200        0     1.43762  -0.36962  -1.86724  L
 H-HO-0.418600        0     1.78203   0.93848  -3.61437  L
 H-H1-0.061500        0    -0.43889   0.3467   -0.72006  L
 H-HO-0.437600        0    -0.98164   2.29923  -0.9467   L
 O-OW--0.834000       0     6.17718   3.80237  -0.37739  L
 H-HW-0.417000        0     5.22277   3.85425  -0.19923  L
 H-HW-0.417000        0     6.45419   3.13331   0.27335  L
 O-OW--0.834000       0     11.60366   11.12654  -1.25322  L
 H-HW-0.417000        0     12.29007   10.97578  -0.58051  L
 H-HW-0.417000        0     12.10614   11.49312  -2.00067  L
 O-OW--0.834000       0     10.4705   8.70704  -1.14873  L
 H-HW-0.417000        0     10.69848   9.66196  -1.15673  L
 H-HW-0.417000        0     11.34767   8.28797  -1.04551  L
 O-OW--0.834000       0     8.23717   7.24235  -11.83015  L
 H-HW-0.417000        0     7.54983   7.5484   -12.4211  L
 H-HW-0.417000        0     7.85298   6.40825  -11.464   L
 O-OW--0.834000       0     17.85689  -8.18131   0.27234  L
 H-HW-0.417000        0     18.69182  -8.59496   0.5074   L
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H-HW-0.417000        0     17.24557  -8.53457   0.94485  L
O-OW--0.834000       0     17.50214  -6.44374  -1.85668  L
H-HW-0.417000        0     17.57183  -7.12352  -1.15667  L
H-HW-0.417000        0     18.04584  -5.73334  -1.50746  L
O-OW--0.834000       0     10.32733   2.51842  -10.14154  L
H-HW-0.417000        0     9.45134   2.81963  -9.81372  L
H-HW-0.417000        0     10.52315   3.19476  -10.80259  L
O-OW--0.834000       0     6.45014  -7.9997   -3.49648  L
H-HW-0.417000        0     5.59556  -8.44546  -3.62001  L
H-HW-0.417000        0     6.23634  -7.06662  -3.71927  L
O-OW--0.834000       0     2.44018  -4.47684  -5.63531  L
H-HW-0.417000        0     2.15325  -4.25441  -6.54948  L
H-HW-0.417000        0     2.59645  -3.58374  -5.25261  L
O-OW--0.834000       0     10.001    5.09113  -11.35554  L
H-HW-0.417000        0     9.10232   4.81406  -11.07604  L
H-HW-0.417000        0     9.80327   5.93795  -11.78152  L
O-OW--0.834000       0     0.35864  -8.32885  -7.97526  L
H-HW-0.417000        0     0.43106  -9.01728  -8.63971  L
H-HW-0.417000        0    -0.00021  -8.82711  -7.2121   L
O-OW--0.834000       0     0.06438  -7.39188  -4.17568  L
H-HW-0.417000        0    -0.49113  -6.90779  -4.80372  L
H-HW-0.417000        0     0.08958  -8.30463  -4.59619  L
O-OW--0.834000       0     3.97372  -9.12797  -3.87029  L
H-HW-0.417000        0     3.22444  -9.6745   -3.55489  L
H-HW-0.417000        0     3.54655  -8.25113  -3.99253  L
O-OW--0.834000       0     0.25242  -4.48846  -3.9385   L
H-HW-0.417000        0     1.06649  -4.3952   -4.46105  L
H-HW-0.417000        0    -0.38369  -4.8233   -4.59444  L
O-OW--0.834000       0     0.2328   -5.61927  -1.50411  H
H-HW-0.417000        0     0.29648  -5.15378  -2.37976  H
H-HW-0.417000        0     0.95566  -4.63454  -0.55987  H
O-OW--0.834000       0     5.81282  -5.55253  -4.33078  L
H-HW-0.417000        0     5.42524  -5.68238  -5.21479  L
H-HW-0.417000        0     5.52327  -4.64953  -4.09536  L
O-OW--0.834000       0    -6.45977  -8.76289   2.12628  L
H-HW-0.417000        0    -6.26802  -7.94829   2.63311  L
H-HW-0.417000        0    -7.04325  -8.44139   1.42625  L
O-OW--0.834000       0     5.09059  -10.63558  -1.58334  L
H-HW-0.417000        0     4.25023  -10.4063  -1.15333  L
H-HW-0.417000        0     4.99441  -10.24487  -2.46249  L
O-OW--0.834000       0     2.65833  -6.81161  -4.14964  L
H-HW-0.417000        0     1.6939   -7.00515  -4.1685   L
H-HW-0.417000        0     2.70711  -5.9508   -4.60558  L
O-OW--0.834000       0     4.72746  -6.74547  -0.2822   L
H-HW-0.417000        0     3.91543  -7.13808  -0.64716  L
H-HW-0.417000        0     4.61315  -5.81675  -0.5745   L
O-OW--0.834000       0     4.6084   -6.16784  -6.71189  L
H-HW-0.417000        0     4.31741  -7.09904  -6.73534  L
H-HW-0.417000        0     3.78345  -5.68009  -6.5716   L
O-OW--0.834000       0     1.89334  -7.22329   5.48973  L
H-HW-0.417000        0     2.05645  -6.28172   5.36782  L
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H-HW-0.417000        0     2.30422  -7.42548   6.34828  L
O-OW--0.834000       0     4.85306  -3.10304  -3.63741  L
H-HW-0.417000        0     4.03643  -2.68136  -3.97819  L
H-HW-0.417000        0     5.07635  -2.54407  -2.87088  L
O-OW--0.834000       0     0.74361  -13.94102  -3.34923  L
H-HW-0.417000        0    -0.13889  -13.71688  -3.70528  L
H-HW-0.417000        0     1.33095  -13.64607  -4.06717  L
O-OW--0.834000       0     3.85486  -4.48826  -1.44787  L
H-HW-0.417000        0     4.2874   -4.18613  -2.26056  L
H-HW-0.417000        0     3.02645  -3.96889  -1.45347  L
O-OW--0.834000       0     2.68628  -9.7741   -0.52522  L
H-HW-0.417000        0     2.24608  -10.29911  -1.21768  L
H-HW-0.417000        0     2.49605  -8.85931  -0.82961  L
O-OW--0.834000       0     0.11932  -11.21734  -7.63384  L
H-HW-0.417000        0     0.03409  -10.75913  -6.74153  L
H-HW-0.417000        0    -0.6745   -11.75403  -7.64273  L
O-OW--0.834000       0     7.51739  -10.63786  -0.37264  L
H-HW-0.417000        0     7.344    -9.68305  -0.40276  L
H-HW-0.417000        0     6.74206  -10.98349  -0.85392  L
O-OW--0.834000       0     3.56922  -4.54605   1.59947  L
H-HW-0.417000        0     3.28933  -5.47201   1.6503   L
H-HW-0.417000        0     2.91723  -4.18395   0.96554  L
O-OW--0.834000       0     1.80313  -2.80576  -2.23411  H
H-HW-0.417000        0     0.82721  -2.86133  -2.24616  H
H-HW-0.417000        0     1.98503  -2.48232  -3.15439  H
O-OW--0.834000       0     9.01618  -8.16905  -4.17721  L
H-HW-0.417000        0     8.06622  -8.17047  -3.92515  L
H-HW-0.417000        0     9.21875  -7.21695  -4.24085  L
O-OW--0.834000       0     4.3521   -8.96664  -6.64653  L
H-HW-0.417000        0     3.81222  -9.67986  -7.04259  L
H-HW-0.417000        0     4.3317   -9.18513  -5.6991   L
O-OW--0.834000       0     1.66658  -3.75775  -8.09455  L
H-HW-0.417000        0     1.3449   -2.8377   -8.19117  L
H-HW-0.417000        0     1.64166  -4.09633  -8.99194  L
O-OW--0.834000       0     2.21094  -1.52246   4.1543   H
H-HW-0.417000        0     1.48637  -2.02634   3.74798  H
H-HW-0.417000        0     2.89194  -2.21611   4.25379  H
O-OW--0.834000       0     1.97802  -12.38877  -5.24339  L
H-HW-0.417000        0     2.32818  -12.13222  -6.10889  L
H-HW-0.417000        0     1.10164  -11.92231  -5.21722  L
O-OW--0.834000       0     6.74679  -7.80093  -7.61372  L
H-HW-0.417000        0     6.26678  -6.98321  -7.41012  L
H-HW-0.417000        0     6.09471  -8.47282  -7.35427  L
O-OW--0.834000       0     2.35158  -7.32103  -1.49301  L
H-HW-0.417000        0     1.63503  -6.6683   -1.37291  L
H-HW-0.417000        0     2.6343   -7.12406  -2.40717  L
O-OW--0.834000       0     1.88917  -10.64955  -3.08407  L
H-HW-0.417000        0     2.10223  -11.51573  -3.47151  L
H-HW-0.417000        0     1.14335  -10.36862  -3.67457  L
O-OW--0.834000       0    -7.81323  -5.52218   0.07246  L
H-HW-0.417000        0    -8.33228  -4.89839   0.60903  L
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H-HW-0.417000        0    -8.2143   -6.37806   0.29378  L
O-OW--0.834000       0     2.79291  -11.04374  -7.61173  L
H-HW-0.417000        0     3.00197  -11.53542  -8.41075  L
H-HW-0.417000        0     1.80956  -10.99853  -7.63921  L
O-OW--0.834000       0    -3.65416  -3.16697  -13.1131  L
H-HW-0.417000        0    -3.22047  -4.02599  -13.07477  L
H-HW-0.417000        0    -3.86045  -3.00243  -12.17307  L
O-OW--0.834000       0     9.33157  -8.08147  -8.38105  L
H-HW-0.417000        0     9.12015  -8.45655  -9.23897  L
H-HW-0.417000        0     8.4391   -7.94077  -7.99428  L
O-OW--0.834000       0     2.11225  -6.91696   2.39037  H
H-HW-0.417000        0     1.91393  -6.25377   3.11789  H
H-HW-0.417000        0     1.3111   -7.4906    2.47239  H
O-OW--0.834000       0    -0.44124  -8.24751  -0.03259  L
H-HW-0.417000        0    -0.12547  -7.40532  -0.38381  L
H-HW-0.417000        0    -0.62009  -8.75736  -0.83938  L
O-OW--0.834000       0     3.86057  -3.72371   4.20635  L
H-HW-0.417000        0     4.05529  -3.87109   3.262    L
H-HW-0.417000        0     3.02923  -4.22107   4.30531  L
O-OW--0.834000       0     1.41163  -4.93102   4.01101  H
H-HW-0.417000        0     1.00537  -4.35376   3.30615  H
H-HW-0.417000        0     0.58777  -5.29245   4.44831  H
O-OW--0.834000       0    -0.86206  -9.40229  -2.60538  L
H-HW-0.417000        0    -0.6017   -8.51147  -2.89607  L
H-HW-0.417000        0    -0.78539  -9.87576  -3.48093  L
C-CW--0.220700       0     8.10715  -10.42636   10.42917  L
H-H4-0.186200        0     9.12655  -10.32253   10.08165  L
C-CT--0.149000       0     12.27629  -3.65094   12.97881  L
H-H1-0.097600        0     12.23227  -2.83204   13.69892  L
H-H1-0.097600        0     11.73908  -4.51271   13.37541  L
H-H1-0.097600        0     13.32318  -3.91904   12.82264  L
H-HC                 0    -6.79541  -9.97944  -7.40166  L
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**IC**

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N-N--0.347900         0    -7.46034   15.26848   3.79296  L
 C-CT--0.263700       -1   -7.38724   13.90613   4.34137  L
 C-C-0.734100          0    -6.57503   13.03123   3.38949  L
 O-O--0.589400         0    -6.95084   12.90185   2.23087  L
 C-CT--0.000700        0    -8.80921   13.31912   4.50501  L
 C-CT-0.039000         0    -9.5897    13.90309   5.6941   L
 C-CT-0.048600         0    -11.01724   13.33081   5.81632  L
 N-N2--0.529502        0    -11.0744   11.92791   6.29121  L
 C-CA-0.807600         0    -10.99145   11.49071   7.53687  L
 N-N2--0.862702        0    -10.69254   12.27017   8.53872  L
 N-N2--0.862702        0    -11.22226   10.23992   7.79943  L
 H-H-0.274700          0    -7.24704   15.39104   2.80273  L
 H-H-0.274700          0    -7.49937   16.0842   4.39198  L
 H-H1-0.156001         0    -6.8826    13.91933   5.30781  L
 H-HC-0.032700         0    -8.73779   12.23951   4.63359  L
 H-HC-0.032700         0    -9.37376   13.50094   3.59135  L
 H-HC-0.028500         0    -9.67148   14.98198   5.55602  L
 H-HC-0.028500         0    -9.04024   13.72096   6.61804  L
 H-H1-0.068701         0    -11.50888   13.39976   4.84365  L
 H-H1-0.068701         0    -11.58491   13.9612   6.50427  L
 H-H-0.345600          0    -11.36322   11.20886   5.63635  L
 H-H-0.447800          0    -10.65662   11.90638   9.47332  L
 H-H-0.447800          0    -10.55483   13.24803   8.36668  L
 H-H-0.447800          0    -11.19046   9.87067   8.72999  L
 H-H-0.447800          0    -11.53775   9.65304   7.02843  L
 N-N--0.415700         0    -5.50005   12.42919   3.89369  L
 C-CT--0.087500       -1   -4.52605   11.63846   3.12702  L
 C-C-0.597300          0    -4.40056   10.23713   3.70539  L
 O-O--0.567900         0    -4.37056   10.08961   4.92925  L
 C-CT-0.298500         0    -3.18885   12.39543   3.01527  L
 C-CT--0.319200        0    -2.52718   12.64375   4.37258  L
 C-CT--0.319200        0    -2.21767   11.6787   2.07571  L
 H-H-0.271900          0    -5.29208   12.55347   4.87114  L
 H-H1-0.096900         0    -4.90787   11.51977   2.11478  L
 H-HC--0.029700        0    -3.39771   13.37219   2.57774  L
 H-HC-0.079100         0    -3.18945   13.20168   5.0312   L
 H-HC-0.079100         0    -1.62027   13.23307   4.22852  L
 H-HC-0.079100         0    -2.25482   11.69939   4.84211  L
 H-HC-0.079100         0    -1.29591   12.25631   1.9942   L
 H-HC-0.079100         0    -2.66241   11.59477   1.08479  L
 H-HC-0.079100         0    -1.97834   10.68573   2.44892  L
 N-N--0.347900         0    -4.41179   9.20677   2.84481  L
 C-CT--0.263700       -1   -4.60168   7.8171    3.29398  L
 C-C-0.734100          0    -3.44913   6.8516    3.09001  L
 O-O--0.589400         0    -2.53073   7.10309   2.32147  L
 C-CT--0.000700        0    -5.97609   7.23521   2.89334  L
 C-CT-0.039000         0    -6.04077   6.15831   1.79293  L    H-H1
48    0.        0.
 C-CT-0.048600         0    -5.40543   6.56171   0.46027  H
 N-N2--0.529500        0    -5.6877    5.59698  -0.59185  H
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 C-CA-0.807600        0    -5.00732   4.45062  -0.81666  H
 N-N2--0.862700       0    -3.72284   4.32285  -0.46488  H
 N-N2--0.862700       0    -5.64463   3.43099  -1.37166  H
 H-H-0.274700         0    -4.40551   9.42366   1.85544  L
 H-H1-0.156000        0    -4.65287   7.86203   4.38229  L
 H-HC-0.032700        0    -6.63757   8.05097   2.63233  L
 H-HC-0.032700        0    -6.40803   6.77774   3.78512  L
 H-HC-0.028500        0    -7.09387   5.94002   1.61669  L
 H-HC-0.028500        0    -5.57845   5.23555   2.1434   L
 H-H1-0.068700        0    -4.32961   6.67223   0.57517  H
 H-H1-0.068700        0    -5.80792   7.52353   0.15976  H
 H-H-0.345600         0    -6.67446   5.48805  -0.85466  H
 H-H-0.447800         0    -3.23599   3.47433  -0.81536  H
 H-H-0.447800         0    -3.17486   5.18489  -0.41435  H
 H-H-0.447800         0    -5.15595   2.60343  -1.81749  H
 H-H-0.447800         0    -6.64978   3.61189  -1.52559  H
 N-N--0.415700        0    -3.53195   5.72837   3.78973  L
 C-CT--0.002400      -1    -2.60303   4.61692   3.73325  L
 C-C-0.597300         0    -3.31166   3.29635   4.05034  L
 O-O--0.567900        0    -4.09516   3.22037   4.99687  L
 C-CT--0.034300       0    -1.47006   4.92776   4.72872  L
 C-CA-0.011800        0    -0.49949   3.80252   5.03355  L
 C-CA--0.125600       0     0.32765   3.26518   4.02949  L
 C-CA--0.125600       0    -0.40451   3.31079   6.34776  L
 C-CA--0.170400       0     1.24111   2.24141   4.3459   L
 C-CA--0.170400       0     0.49357   2.27553   6.65792  L
 C-CA--0.107200       0     1.32068   1.74156   5.65571  L
 H-H-0.271900         0    -4.25276   5.67695   4.50158  L
 H-H1-0.097800        0    -2.17965   4.54934   2.72951  L
 H-HC-0.029500        0    -1.92196   5.25218   5.66814  L
 H-HC-0.029500        0    -0.89508   5.77165   4.3445   L
 H-HA-0.133000        0     0.26748   3.64395   3.02035  L
 H-HA-0.133000        0    -1.03628   3.72424   7.1178   L
 H-HA-0.143000        0     1.90096   1.82992   3.59617  L
 H-HA-0.143000        0     0.53633   1.88183   7.66102  L
 H-HA-0.129700        0     2.01928   0.94611   5.88245  L
 N-N--0.415700        0    -3.04213   2.26691   3.24431  L
 C-CT-0.033700       -1    -3.81985   1.02886   3.20323  L
 C-C-0.597300         0    -2.93912  -0.23594   3.33474  L
 O-O--0.567900        0    -2.80743  -1.00563   2.38371  L
 C-CT--0.182500       0    -4.65604   1.0962    1.91922  L
 H-H-0.271900         0    -2.39347   2.41542   2.48731  L
 H-H1-0.082300        0    -4.5252    1.00931   4.03176  L
 H-HC-0.060300        0    -4.00737   1.22881   1.05331  L
 H-HC-0.060300        0    -5.35331   1.93368   1.97169  L
 H-HC-0.060300        0    -5.22458   0.17953   1.80462  L
 N-N--0.254800        0    -2.30719  -0.49299   4.49378  L
 C-CT--0.026600       0    -1.50526  -1.69352   4.71286  L    H-H2
98    0.        0.
 C-C-0.589600         0    -2.32732  -2.99318   4.52967  H
 O-O--0.574800        0    -3.38633  -3.23545   5.08965  H
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 C-CT--0.007000       0    -0.91365  -1.56057   6.12135  L
 C-CT-0.018900        0    -1.81463  -0.52991   6.79777  L
 C-CT-0.019200        0    -2.19798   0.38343   5.6421   L
 H-H1-0.064100        0    -0.68322  -1.68853   3.99835  L
 H-HC-0.025300        0     0.10126  -1.16604   6.05199  L
 H-HC-0.025300        0    -0.91596  -2.50868   6.66051  L
 H-HC-0.021300        0    -1.3031    0.01035   7.59385  L
 H-HC-0.021300        0    -2.70972  -1.02334   7.17155  L
 H-H1-0.039100        0    -3.11191   0.92722   5.86322  L
 H-H1-0.039100        0    -1.39947   1.08865   5.44231  L
 N-N--0.415700        0    -1.72696  -3.84194   3.65602  H
 C-CT--0.024900       0    -2.12177  -5.22316   3.50085  H
 C-C-0.597300         0    -1.68056  -6.01867   4.73917  L    H-H1
111   0.        0.
 O-O--0.567900        0    -0.48227  -6.03328   5.03608  L
 C-CT-0.211700        0    -1.46569  -5.83426   2.26819  H
 O-OH--0.654600       0    -1.82697  -5.20131   1.06701  H
 H-H-0.271900         0    -0.78956  -3.60176   3.3504   H
 H-H1-0.084300        0    -3.2056   -5.2581    3.39026  H
 H-H1-0.035200        0    -1.77614  -6.88224   2.2015   H
 H-H1-0.035200        0    -0.36676  -5.80957   2.39695  H
 H-HO-0.427500        0    -1.43774  -4.27004   1.11897  H
 N-N--0.254800        0    -2.60179  -6.66374   5.47901  L
 C-CT--0.026600       0    -2.29346  -7.48781   6.64053  L
 C-C-0.589600         0    -1.77764  -8.85425   6.17154  L
 O-O--0.574800        0    -2.3824   -9.89126   6.42937  L
 C-CT--0.007000       0    -3.61617  -7.57881   7.40769  L
 C-CT-0.018900        0    -4.65869  -7.58513   6.29383  L
 C-CT-0.019200        0    -4.0301   -6.69391   5.22529  L
 H-H1-0.064100        0    -1.54017  -7.00674   7.26386  L
 H-HC-0.025300        0    -3.73343  -6.68326   8.01067  L
 H-HC-0.025300        0    -3.68839  -8.46177   8.04352  L
 H-HC-0.021300        0    -5.60928  -7.18133   6.63643  L
 H-HC-0.021300        0    -4.78628  -8.59602   5.90374  L
 H-H1-0.039100        0    -4.2243   -7.10986   4.23669  L
 H-H1-0.039100        0    -4.43438  -5.68632   5.30511  L
 N-N--0.415700        0    -0.65002  -8.84639   5.46502  L
 C-CT--0.038900      -1    -0.15701  -9.98713   4.6919   L
 C-C-0.597300         0     1.34561  -10.24497   4.9133   L
 O-O--0.567900        0     2.10176  -10.52061   3.98024  L
 C-CT-0.365400        0    -0.48958  -9.8452    3.1889   L
 O-OH--0.676100       0    -0.01619  -8.62338   2.65541  L
 C-CT--0.243800       0    -1.99378  -9.89519   2.91729  L
 H-H-0.271900         0    -0.22273  -7.94649   5.27966  L
 H-H1-0.100700        0    -0.65336  -10.89742   5.03206  L
 H-H1-0.004300        0    -0.03021  -10.67061   2.64377  L
 H-HC-0.064200        0    -2.49505  -9.04063   3.36961  L
 H-HC-0.064200        0    -2.40899  -10.81507   3.33037  L
 H-HC-0.064200        0    -2.17159  -9.88353   1.8417   L
 H-HO-0.410200        0    -0.24865  -8.63911   1.69939  L
 N-N--0.415700        0     1.79675  -10.1642   6.169    L
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C-CT--0.025200       -1    3.19383  -10.32521   6.59399  L
C-C-0.597300         0     3.74323  -9.10769   7.36869  L
O-O--0.567900        0     3.03835  -8.11615   7.57633  L
H-H-0.271900         0     1.11595  -9.96426   6.88648  L
H-H1-0.069800        0     3.82924  -10.47932   5.7232   L
H-H1-0.069800        0     3.27578  -11.21031   7.22068  L
N-N--0.415700        0     5.01353  -9.16      7.78755  L
C-CT--0.058100       -1    5.71153  -8.08039   8.51983  L
C-C-0.597300         0     5.89974  -6.80997   7.6712   L
O-O--0.567900        0     6.17214  -6.88102   6.47459  L
C-CT--0.007400       0     7.07354  -8.59217   9.01399  L
C-CC-0.186800        0     6.99425  -9.70393   10.03393  L
N-NB--0.543200       0     5.85172  -10.09077   10.73726  L
C-CR-0.163500        0     6.24286  -11.07139   11.56467  L
N-NA--0.279500       0     7.55556  -11.32108   11.40971  L
H-H-0.271900         0     5.53035  -10.00535   7.6058   L
H-H1-0.136000        0     5.10943  -7.81704   9.39021  L
H-HC-0.036700        0     7.61332  -7.76304   9.4732   L
H-HC-0.036700        0     7.65726  -8.93773   8.15932  L
H-H-0.333900         0     8.08399  -12.00845   11.93193  L
H-H5-0.143500        0     5.59316  -11.58175   12.26462  L
N-N--0.415700        0     5.79359  -5.64334   8.31622  L
C-CT--0.051800       0     5.99872  -4.31468   7.72538  L
C-C-0.597300         0     7.42894  -4.1319    7.19041  L
O-O--0.567900        0     8.38745  -4.19087   7.96596  L
C-CT--0.110200       0     5.71113  -3.26567   8.81739  L
C-CT-0.353100        0     5.94229  -1.8015    8.39349  L
C-CT--0.412100       0     4.92197  -1.29956   7.37334  L
C-CT--0.412100       0     5.8691   -0.91071   9.6309   L
H-H-0.271900         0     5.59813  -5.68662   9.30208  L
H-H1-0.092200        0     5.29481  -4.18363   6.90096  L
H-HC-0.045700        0     6.36701  -3.47774   9.66389  L
H-HC-0.045700        0     4.68767  -3.37951   9.1619   L
H-HC--0.036100       0     6.93457  -1.69286   7.96497  L
H-HC-0.100000        0     3.91815  -1.31976   7.78718  L
H-HC-0.100000        0     4.95746  -1.91066   6.47154  L
H-HC-0.100000        0     5.15264  -0.2742    7.09755  L
H-HC-0.100000        0     4.88716  -0.99979   10.0935  L
H-HC-0.100000        0     6.05163   0.12461   9.34922  L
H-HC-0.100000        0     6.63246  -1.2138    10.34771  L
N-N--0.415700        0     7.56723  -3.80617   5.90239  L
C-CT--0.058100       -1    8.84853  -3.42406   5.29183  L
C-C-0.597300         0     8.96968  -1.91601   5.06692  L
O-O--0.567900        0     7.99324  -1.16185   5.10792  L
C-CT--0.007400       0     9.09363  -4.22576   4.00441  L
C-CC-0.186800        0     8.30968  -3.74274   2.81569  L
N-NB--0.543200       0     8.75155  -2.79283   1.89411  L
C-CW--0.220700       0     7.0743   -4.18336   2.45436  L
C-CR-0.163500        0     7.77969  -2.7135    0.96951  L
N-NA--0.279500       0     6.7534   -3.51405   1.29482  L
H-H-0.271900         0     6.72919  -3.75002   5.33765  L
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H-H1-0.136000        0     9.65215  -3.69273   5.97587  L
H-HC-0.036700        0     8.86733  -5.27808   4.18276  L
H-HC-0.036700        0     10.14992  -4.16207   3.74447  L
H-H4-0.186200        0     6.47353  -4.92201   2.96785  L
H-H-0.333900         0     5.88772  -3.61271   0.76668  L
H-H5-0.143500        0     7.80913  -2.09827   0.0811   L
N-N--0.415700        0     10.20623  -1.47811   4.84461  L
C-CT--0.087500       -1    10.59331  -0.06936   4.69256  L
C-C-0.597300         0     9.84877   0.68542   3.59161  L
O-O--0.567900        0     9.52585   1.84987   3.79544  L
C-CT-0.298500        0     12.11839   0.07182   4.52671  L
C-CT--0.319200       0     12.83616  -0.30913   5.82748  L
C-CT--0.319200       0     12.68251  -0.78007   3.38415  L
H-H-0.271900         0     10.94122  -2.178     4.85     L
H-H1-0.096900        0     10.32941   0.44033   5.6183   L
H-HC--0.029700       0     12.34469   1.11542   4.31521  L
H-HC-0.079100        0     12.6747  -1.36128   6.06575  L
H-HC-0.079100        0     12.47006   0.30439   6.65008  L
H-HC-0.079100        0     13.90712  -0.13821   5.71902  L
H-HC-0.079100        0     12.49414  -1.8391    3.55913  L
H-HC-0.079100        0     13.75908  -0.63961   3.31957  L
H-HC-0.079100        0     12.2431  -0.47802   2.43535  L
N-N--0.415700        0     9.53928   0.0639    2.45068  L
C-CT--0.025200       -1    8.75234   0.68906   1.38135  L
C-C-0.597300         0     7.31355   0.99489   1.81394  L
O-O--0.567900        0     6.83676   2.10936   1.60354  L
H-H-0.271900         0     9.74955  -0.926     2.37523  L
H-H1-0.069800        0     8.72423   0.03192   0.51278  L
H-H1-0.069800        0     9.22238   1.62507   1.09033  L
N-N--0.415700        0     6.63426   0.03706   2.45262  L
C-CT--0.025200       0     5.31833   0.23469   3.07531  L
C-C-0.597300         0     5.33035   1.34724   4.13261  L
O-O--0.567900        0     4.56214   2.30741   4.0567   L
H-H-0.271900         0     7.09891  -0.8521    2.59298  L
H-H1-0.069800        0     5.00543  -0.6936    3.55198  L
H-H1-0.069800        0     4.58757   0.49021   2.30765  L
N-N--0.415700        0     6.2455    1.25512   5.10272  L
C-CT-0.033700        -1    6.45486   2.26416   6.14827  L
C-C-0.597300         0     6.7656    3.65827   5.58498  L
O-O--0.567900        0     6.28517   4.6579    6.11335  L
C-CT--0.182500       0     7.56707   1.77389   7.06783  L
H-H-0.271900         0     6.83867   0.42988   5.0957   L
H-H1-0.082300        0     5.53275   2.34401   6.72275  L
H-HC-0.060300        0     7.3029    0.78014   7.4165   L
H-HC-0.060300        0     7.67051   2.44678   7.91981  L
H-HC-0.060300        0     8.51238   1.72636   6.52609  L
N-N--0.347900        0     7.55326   3.74178   4.50872  L
C-CT--0.263700       -1    7.80779   4.97553   3.76091  L
C-C-0.734100         0     6.5257    5.62048   3.22152  L
O-O--0.589400        0     6.44056   6.83925   3.28641  L
C-CT--0.000700       0     8.92424   4.73276   2.73025  L
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C-CT-0.039000        0     9.22015   5.88447   1.75154  L
C-CT-0.048600        0     8.29314   5.7654    0.54077  L
N-N2--0.529500       0     8.7579    6.51109  -0.63139  L
C-CA-0.807600        0     8.63527   6.11278  -1.88141  L
N-N2--0.862700       0     7.94119   5.07428  -2.23391  L
N-N2--0.862700       0     9.2346    6.75734  -2.82993  L
H-H-0.274700         0     7.98128   2.88219   4.17585  L
H-H1-0.156000        0     8.19962   5.70453   4.46873  L
H-HC-0.032700        0     8.71096   3.82557   2.16687  L
H-HC-0.032700        0     9.83732   4.53698   3.2904   L
H-HC-0.028500        0     10.25032   5.78045   1.4075   L
H-HC-0.028500        0     9.10678   6.8548    2.23684  L
H-H1-0.068700        0     7.28279   6.08536   0.79451  L
H-H1-0.068700        0     8.28218   4.7119    0.27257  L
H-H-0.345600         0     9.29233   7.36582  -0.50809  L
H-H-0.447800         0     7.93317   4.82118  -3.21385  L
H-H-0.447800         0     7.34325   4.60269  -1.55827  L
H-H-0.447800         0     9.23059   6.34153  -3.75114  L
H-H-0.447800         0     9.77882   7.56803  -2.55946  L
N-N--0.415700        0     5.52235   4.86827   2.75561  L
C-CT--0.038900      -1     4.18785   5.42826   2.42744  L
C-C-0.597300         0     3.54678   6.08811   3.64716  L
O-O--0.567900        0     3.08577   7.21943   3.54536  L
C-CT-0.365400        0     3.22638   4.37922   1.84609  L
O-OH--0.676100       0     3.8465    3.65915   0.81228  L
C-CT--0.243800       0     1.98475   5.01334   1.22065  L
H-H-0.271900         0     5.65626   3.86599   2.69727  L
H-H1-0.100700        0     4.3248    6.20412   1.67325  L
H-H1-0.004300        0     2.92609   3.68463   2.62756  L
H-HC-0.064200        0     1.41304   5.54901   1.97765  L
H-HC-0.064200        0     1.35427   4.23934   0.78394  L
H-HC-0.064200        0     2.28111   5.71353   0.43833  L
H-HO-0.410200        0     3.40251   2.79691   0.75404  L
N-N--0.415700        0     3.5332    5.41557   4.80566  L
C-CT-0.033700       -1     3.07274   6.00849   6.06703  L
C-C-0.597300         0     3.82228   7.30181   6.40877  L
O-O--0.567900        0     3.1827    8.3185    6.63201  L
C-CT--0.182500       0     3.12947   4.97156   7.18714  L
H-H-0.271900         0     3.92927   4.48442   4.81731  L
H-H1-0.082300        0     2.02677   6.28397   5.93243  L
H-HC-0.060300        0     2.5774    4.08289   6.88744  L
H-HC-0.060300        0     2.67846   5.39105   8.08678  L
H-HC-0.060300        0     4.15943   4.70245   7.40183  L
N-N--0.415700        0     5.15747   7.2774    6.41466  L
C-CT--0.051800      -1     6.02268   8.43985   6.64051  L
C-C-0.597300         0     5.71556   9.60696   5.70682  L
O-O--0.567900        0     5.53432   10.72752   6.16829  L
C-CT--0.110200       0     7.49064   7.98011   6.52592  L
C-CT-0.353100        0     8.53989   9.07983   6.7813   L
C-CT--0.412100       0     8.54386   9.54238   8.23809  L
C-CT--0.412100       0     9.93371   8.54048   6.44696  L
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H-H-0.271900          0      5.59116   6.37941   6.23145  L
H-H1-0.092200         0      5.84443   8.79344   7.65698  L
H-HC-0.045700         0      7.64585   7.59746   5.51918  L
H-HC-0.045700         0      7.66052   7.16009   7.22536  L
H-HC--0.036100        0      8.34794   9.93501   6.13446  L
H-HC-0.100000         0      9.31854   10.29481   8.38564  L
H-HC-0.100000         0      8.72465   8.70075   8.90614  L
H-HC-0.100000         0      7.58543   9.99737   8.48558  L
H-HC-0.100000         0      10.16021   7.68125   7.0782   L
H-HC-0.100000         0      10.67285   9.32291   6.61797  L
H-HC-0.100000         0      9.96635   8.2472    5.39771  L
N-N--0.415700         0      5.68744   9.34189   4.40436  L
C-CT--0.002400        -1     5.40031   10.32806   3.37406  L
C-C-0.597300          0      4.01459   10.95616   3.54936  L
O-O--0.567900         0      3.87872   12.17498   3.57739  L
C-CT--0.034300        0      5.57211   9.67251   1.99089  L
C-CA-0.011800         0      5.63557   10.63863   0.82058  L
C-CA--0.125600        0      6.88187   10.99143   0.26556  L
C-CA--0.125600        0      4.45555   11.16699   0.26296  L
C-CA--0.170400        0      6.94724   11.86866  -0.83208  L
C-CA--0.170400        0      4.51961   12.04543  -0.83338  L
C-CA--0.107200        0      5.76565   12.3981  -1.38019  L
H-H-0.271900          0      5.85463   8.38726   4.10889  L
H-H1-0.097800         0      6.12713   11.13719   3.45913  L
H-HC-0.029500         0      4.76071   8.96278   1.82081  L
H-HC-0.029500         0      6.50149   9.10246   1.99293  L
H-HA-0.133000         0      7.79596   10.59274   0.68017  L
H-HA-0.133000         0      3.49308   10.9054   0.67626  L
H-HA-0.143000         0      7.90682   12.14246  -1.24869  L
H-HA-0.143000         0      3.60848   12.45003  -1.25281  L
H-HA-0.129700         0      5.81287   13.07906  -2.2182   L
N-N--0.415700         0      2.98599   10.11892   3.68195  L
C-CT-0.014300         -1     1.60149   10.55376   3.82531  L
C-C-0.597300          0      1.28886   11.14319   5.23122  L
O-O--0.567900         0      0.28589   11.83439   5.38198  L
C-CT--0.204100        0      0.66698   9.38379   3.45261  L
C-C-0.713000          0      0.7522    8.97183   1.98527  L
O-O--0.593100         0      1.49498   9.49809   1.17747  L
N-N--0.919100         0     -0.03064   8.01722   1.55097  L
H-H-0.271900          0      3.17508   9.12496   3.62365  L
H-H1-0.104800         0      1.42387   11.36549   3.11635  L
H-HC-0.079700         0     -0.35904   9.67346   3.6656   L
H-HC-0.079700         0      0.91082   8.52155   4.068    L
H-H-0.419600          0      0.08642   7.81079   0.57842  L
H-H-0.419600          0     -0.79991   7.62531   2.08013  L
N-N--0.415700         0      2.09512   10.86692   6.26565  L
C-CT--0.027500        -1     2.11181   11.55097   7.57589  L
C-C-0.597300          0      2.75868   12.94668   7.46097  L
N-N--0.415700         0      3.95726   13.03055   6.86366  L
C-CT--0.149000        -1     4.74079   14.24687   6.64809  L
O-O--0.567900         0      2.16914   13.92681   7.91283  L
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C-CT--0.005000       0     2.84205   10.66963   8.59845  L
C-C*--0.141500       0     3.16306   11.30917   9.91301  L
C-CW--0.163800       0     2.30283   11.48624   10.94113  L
C-CB-0.124300        0     4.43652   11.87926   10.34606  L
N-NA--0.341800       0     2.95898   12.11632   11.98373  L
C-CN-0.138000        0     4.2777    12.37499   11.67316  L
C-CA--0.238700       0     5.70643   12.03603   9.74804  L
C-CA--0.260100       0     5.32697   12.98157   12.37993  L
C-CA--0.197200       0     6.76811   12.64392   10.4464  L
C-CA--0.113400       0     6.5816    13.11354   11.75948  L
H-H-0.271900         0     2.82269   10.18184   6.10271  L
H-H-0.271900         0     4.35032   12.16343   6.51568  L
H-H1-0.112300        0     1.08916   11.70561   7.91735  L
H-HC-0.033900        0     3.78635   10.34223   8.16569  L
H-HC-0.033900        0     2.23942   9.77911   8.78215  L
H-H4-0.206200        0     1.26265   11.18769   10.92966  L
H-H-0.341200         0     2.52027   12.39001   12.85046  L
H-HA-0.170000        0     5.84743   11.70064   8.73094  L
H-HA-0.157200        0     5.16913   13.35278   13.38114  L
H-HA-0.144700        0     7.72914   12.76527   9.96627  L
H-HA-0.141700        0     7.399     13.58906   12.28473  L
H-H1-0.097600        0     5.21507   14.5481   7.58342  L
H-H1-0.097600        0     4.0846    15.04977   6.30703  L
H-H1-0.097600        0     5.50399   14.06314   5.89086  L
N-N--0.415700        0    -3.7683    12.27976   8.44728  L
C-CT--0.002400      -1    -3.39904   10.90999   8.09272  L
C-C-0.597300         0    -4.51412   9.918     8.44789  L
O-O--0.567900        0    -5.19015   10.07935   9.46338  L
C-CT--0.034300       0    -2.08342   10.57275   8.80732  L
C-CA-0.011800        0    -1.51356   9.20631   8.48235  L
C-CA--0.125600       0    -0.95471   8.9625    7.21442  L
C-CA--0.125600       0    -1.51027   8.18814   9.45495  L
C-CA--0.170400       0    -0.38282   7.71163   6.92584  L
C-CA--0.170400       0    -0.93118   6.93948   9.16766  L
C-CA--0.107200       0    -0.36372   6.70275   7.90373  L
H-H-0.271900         0    -4.44917   12.37697   9.19133  L
H-H-0.271900         0    -3.09584   13.0175   8.27738  L
H-H1-0.097800        0    -3.22381   10.86507   7.01805  L
H-HC-0.029500        0    -2.23766   10.64904   9.88508  L
H-HC-0.029500        0    -1.33587   11.31899   8.53197  L
H-HA-0.133000        0    -0.94287   9.74441   6.4682   L
H-HA-0.133000        0    -1.93408   8.36916   10.43271  L
H-HA-0.143000        0     0.06345   7.53631   5.95934  L
H-HA-0.143000        0    -0.90927   6.17157   9.92693  L
H-HA-0.129700        0     0.10063   5.75335   7.68552  L
N-N--0.415700        0    -4.7299    8.91745   7.59314  L
C-CT--0.059700      -1    -5.7369    7.86373   7.74979  L
C-C-0.597300         0    -5.08077   6.50817   7.4742   L
O-O--0.567900        0    -4.47103   6.3398    6.4182   L
C-CT-0.130300        0    -6.96175   8.10046   6.82846  L
C-CT--0.043000       0    -7.76469   9.37608   7.18458  L
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C-CT--0.320400       0    -7.92699   6.90208   6.92623  L
C-CT--0.066000       0    -7.27911   10.66196   6.50469  L
H-H-0.271900         0    -4.16894   8.90189   6.74918  L
H-H1-0.086900        0    -6.08727   7.857     8.78266  L
H-HC-0.018700        0    -6.6265    8.17267   5.79319  L
H-HC-0.023600        0    -7.7717    9.51671   8.26625  L
H-HC-0.023600        0    -8.79795   9.2432    6.86532  L
H-HC-0.088200        0    -8.24127   6.74412   7.95873  L
H-HC-0.088200        0    -7.45996   5.99086   6.54984  L
H-HC-0.088200        0    -8.80972   7.07182   6.31273  L
H-HC-0.018600        0    -6.28381   10.9392   6.83577  L
H-HC-0.018600        0    -7.95778   11.47325   6.76186  L
H-HC-0.018600        0    -7.26833   10.5274   5.4241   L
N-N--0.415700       -1    -5.22978   5.54292   8.39294  L
C-CT--0.051800       0    -4.63789   4.21103   8.26819  L
C-C-0.597300         0    -5.75362   3.1718    8.27187  L
O-O--0.567900        0    -6.47902   3.04517   9.2576   L
C-CT--0.110200       0    -3.5954    4.00265   9.38491  L
C-CT-0.353100        0    -2.78349   2.69249   9.26865  L
C-CT--0.412100       0    -1.43503   2.85066   9.97883  L
C-CT--0.412100       0    -3.47126   1.47912   9.89969  L
H-H-0.271900         0    -5.78819   5.72742   9.21252  L
H-H1-0.092200        0    -4.11188   4.13699   7.31615  L
H-HC-0.045700        0    -4.08218   4.04632   10.36052  L
H-HC-0.045700        0    -2.90176   4.84097   9.32521  L
H-HC--0.036100       0    -2.59232   2.47563   8.21846  L
H-HC-0.100000        0    -0.8539    1.93441   9.87955  L
H-HC-0.100000        0    -1.59622   3.06178   11.03673  L
H-HC-0.100000        0    -0.8724    3.6693    9.53232  L
H-HC-0.100000        0    -3.73788   1.69441   10.93481  L
H-HC-0.100000        0    -2.80382   0.61902   9.87344  L
H-HC-0.100000        0    -4.3728    1.21873   9.35045  L
N-N--0.347900        0    -5.86291   2.41916   7.17643  L
C-CT--0.263700      -1    -6.78996   1.29824   7.03353  L
C-C-0.734100         0    -6.03235  -0.0251    6.89276  L
O-O--0.589400        0    -5.18467  -0.16183   6.02038  L
C-CT--0.000700       0    -7.69577   1.51      5.81562  L
C-CT-0.039000        0    -8.57554   0.26546   5.60896  L
C-CT-0.048600        0    -9.68118   0.49938   4.60292  L
N-N2--0.529500       0    -9.16321   0.698     3.24197  L
C-CA-0.807600        0    -9.15423   1.80226   2.52803  L
N-N2--0.862700       0    -9.76868   2.89956   2.85253  L
N-N2--0.862700       0    -8.49653   1.79846   1.41631  L
H-H-0.274700         0    -5.23788   2.62417   6.39998  L
H-H1-0.156000        0    -7.42357   1.22853   7.9203   L
H-HC-0.032700        0    -7.08895   1.67851   4.92361  L
H-HC-0.032700        0    -8.3212    2.38521   5.98482  L
H-HC-0.028500        0    -9.03812  -0.01451   6.55664  L
H-HC-0.028500        0    -7.96736  -0.56043   5.24935  L
H-H1-0.068700        0    -10.23011   1.36876   4.94615  L
H-H1-0.068700        0    -10.34165  -0.36736   4.61275  L
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 H-H-0.345600          0    -8.72039  -0.08021   2.76215  L
 H-H-0.447800          0    -9.72251   3.64513   2.16183  L
 H-H-0.447800          0    -10.54631   2.84581   3.51717  L
 H-H-0.447800          0    -8.52006   2.65758   0.86634  L
 H-H-0.447800          0    -8.1116    0.91311   1.09445  L
 N-N--0.415700         0    -6.38428  -1.02838   7.68973  L
 C-CT--0.059700        -1   -5.97729  -2.42218   7.45063  L
 C-C-0.597300          0    -6.8912   -3.0385    6.38246  L
 O-O--0.567900         0    -8.10022  -2.82643   6.41075  L
 C-CT-0.130300         0    -6.13949  -3.21685   8.76883  L
 C-CT--0.043000        0    -5.38568  -2.60688   9.97522  L
 C-CT--0.320400        0    -5.72751  -4.68318   8.57787  L
 C-CT--0.066000        0    -3.90235  -2.29458   9.74008  L
 H-H-0.271900          0    -7.15756  -0.86562   8.3232   L
 H-H1-0.086900         0    -4.94184  -2.46389   7.11042  L
 H-HC-0.018700         0    -7.1989   -3.21734   9.0343   L
 H-HC-0.023600         0    -5.46562  -3.28954   10.82213  L
 H-HC-0.023600         0    -5.88225  -1.68133   10.27005  L
 H-HC-0.088200         0    -6.40932  -5.18193   7.88834  L
 H-HC-0.088200         0    -5.78691  -5.2115    9.52787  L
 H-HC-0.088200         0    -4.71492  -4.72658   8.1818   L
 H-HC-0.018600         0    -3.44252  -1.99738   10.6828  L
 H-HC-0.018600         0    -3.81387  -1.46948   9.03797  L
 H-HC-0.018600         0    -3.378    -3.16378   9.34668  L
 N-N--0.516300         0    -6.35463  -3.84209   5.46762  L
 C-CT-0.039700         -1   -7.14347  -4.3962    4.35881  L
 C-C-0.536600          0    -7.22276  -5.92929   4.3283   L
 O-O--0.581900         0    -6.50569  -6.58494   3.57484  L
 C-CT-0.056000         0    -6.60226  -3.81914   3.02477  L    H-HC
485   0.        0.
 C-CT-0.013600         0    -6.77464  -2.2924    2.91599  H
 C-C-0.805400          0    -7.01492  -1.70902   1.52703  H
 O-O2--0.818800        0    -6.17268  -1.96654   0.53486  H
 O-O2--0.818800        0    -7.93929  -0.94163   1.33517  H
 H-H-0.293600          0    -5.34224  -3.87934   5.42197  L
 H-H1-0.110500         0    -8.17847  -4.0622    4.42807  L
 H-HC--0.017300        0    -7.14755  -4.28191   2.20989  L
 H-HC--0.017300        0    -5.54686  -4.07131   2.90594  L
 H-HC--0.042500        0    -5.89203  -1.82595   3.36521  H
 H-HC--0.042500        0    -7.65029  -1.992     3.48864  H
 N-N--0.516300         0    -8.11762  -6.52119   5.12321  L
 C-CT-0.038100         -1   -8.34425  -7.96812   5.22979  L
 C-C-0.536600          0    -9.49063  -8.48087   4.33491  L
 O-O--0.581900         0    -10.67748  -8.37314   4.62619  L
 C-CT--0.030300        0    -8.51327  -8.39664   6.69845  L
 C-C-0.799400          0    -9.7124   -7.772     7.4095   L
 O-O2--0.801400        0    -10.025   -6.59423   7.12933  L
 O-O2--0.801400        0    -10.29204  -8.43461   8.29849  L
 H-H-0.293600          0    -8.70767  -5.96614   5.73508  L
 H-H1-0.088000         0    -7.4366   -8.46895   4.89148  L
 H-HC--0.012200        0    -7.6129   -8.13024   7.25199  L
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H-HC--0.012200       0    -8.60662  -9.48371   6.72893  L
N-N--0.415700        0    -9.10366  -9.08411   3.21538  L
C-CT--0.038900       -1   -9.96345  -9.61808   2.14142  L
C-C-0.597300         0    -9.41772  -10.92843   1.55799  L
O-O--0.567900        0    -10.05685  -11.54045   0.69991  L
C-CT-0.365400        0    -10.09198  -8.57422   1.01215  L
O-OH--0.676100       0    -8.82274  -8.15361   0.55343  L
C-CT--0.243800       0    -10.82733  -7.30621   1.44438  L
H-H-0.271900         0    -8.11209  -9.02207   3.02129  L
H-H1-0.100700        0    -10.95593  -9.82481   2.54     L
H-H1-0.004300        0    -10.64311  -9.01368   0.17987  L
H-HC-0.064200        0    -10.2388  -6.76863   2.18779  L
H-HC-0.064200        0    -11.79401  -7.5608    1.87752  L
H-HC-0.064200        0    -10.9709  -6.65248   0.58463  L
H-HO-0.410200        0    -8.60394  -8.73174  -0.22279  L
N-N--0.516300        0    -8.24925  -11.37606   2.02997  L
C-CT-0.038100        -1   -7.44399  -12.46541   1.47936  L
C-C-0.536600         0    -7.08777  -13.51467   2.56571  L
N-N--0.415700        0    -8.11434  -14.14309   3.15698  L
C-CT--0.149000       -1   -7.98798  -15.15951   4.20961  L
O-O--0.581900        0    -5.92408  -13.76354   2.88214  L
C-CT--0.030300       0    -6.21882  -11.8421   0.78582  L
C-C-0.799400         0    -5.61302  -12.77742  -0.25057  L
O-O2--0.801400       0    -4.37535  -12.96149  -0.25483  L
O-O2--0.801400       0    -6.38927  -13.23772  -1.11914  L
H-H-0.293600         0    -7.7719   -10.77573   2.68727  L
H-H-0.271900         0    -9.03734  -13.86058   2.86472  L
H-H1-0.088000        0    -8.03182  -12.9864   0.72478  L
H-HC--0.012200       0    -5.47115  -11.55347   1.52697  L
H-HC--0.012200       0    -6.5289   -10.9393   0.25728  L
H-H1-0.097600        0    -7.43166  -16.01843   3.82911  L
H-H1-0.097600        0    -8.9748   -15.48945   4.53769  L
H-H1-0.097600        0    -7.44832  -14.74279   5.06223  L
N-N--0.347900        0    -3.39764  -14.50733   1.94942  L
C-CT--0.263700       -1   -2.23814  -14.88617   2.7753   L
C-C-0.734100         0    -2.21195  -14.06434   4.09112  L
N-N--0.415700        0    -3.38218  -13.88421   4.72739  L
C-CT--0.149000       -1   -3.5797   -13.21021   6.02045  L
O-O--0.589400        0    -1.15799  -13.60743   4.52657  L
C-CT--0.000700       0    -0.94855  -14.74612   1.94039  L
C-CT-0.039000        0    -0.97945  -15.57997   0.63648  L
C-CT-0.048600        0    -0.7213   -14.75211  -0.63005  L
N-N2--0.529500       0    -1.65806  -13.61677  -0.77678  L
C-CA-0.807600        0    -1.35126  -12.38148  -1.11823  L
N-N2--0.862700       0    -0.16252  -12.03243  -1.49152  L
N-N2--0.862700       0    -2.258    -11.45845  -1.0943   L
H-H-0.271900         0    -4.20584  -14.20053   4.23381  L
H-H-0.274700         0    -3.29564  -13.92858   1.11902  L
H-H-0.274700         0    -4.34491  -14.56867   2.31752  L
H-H1-0.156000        0    -2.33503  -15.93138   3.06982  L
H-HC-0.032700        0    -0.10321  -15.08486   2.54201  L
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H-HC-0.032700        0    -0.78132  -13.69082   1.71786  L
H-HC-0.028500        0    -1.93352  -16.09575   0.52484  L
H-HC-0.028500        0    -0.20989  -16.35032   0.70014  L
H-H1-0.068700        0    -0.81102  -15.40328  -1.50212  L
H-H1-0.068700        0     0.30812  -14.39181  -0.58939  L
H-H-0.345600         0    -2.65704  -13.75651  -0.65637  L
H-H-0.447800         0    -0.06118  -11.12397  -1.92303  L
H-H-0.447800         0     0.39768  -12.79736  -1.851    L
H-H-0.447800         0    -2.03888  -10.55425  -1.49411  L
H-H-0.447800         0    -3.18789  -11.7633  -0.81567  L
H-H1-0.097600        0    -4.5338   -13.50768   6.45703  L
H-H1-0.097600        0    -3.57401  -12.12843   5.87397  L
H-H1-0.097600        0    -2.77159  -13.47369   6.70576  L
N-N--0.415700        0    -0.24979  -8.93083   11.52223  L
C-CT--0.149000      -1    -0.11177  -8.0516    10.35503  L
C-C-0.597300         0    -1.04225  -6.84434   10.51639  L
N-N--0.415700        0    -2.35494  -7.08631   10.49611  L
C-CT--0.149000       0    -3.38138  -6.10698   10.83593  L
O-O--0.567900        0    -0.57072  -5.73551   10.76842  L
C-CT--0.015200       0    -0.27185  -8.88406   9.07741  L
C-CA--0.001100       0     0.47727  -10.21299   9.07894  L
C-CA--0.190600       0     1.76569  -10.31943   9.64868  L
C-CA--0.190600       0    -0.12709  -11.35656   8.51945  L
C-CA--0.234100       0     2.43277  -11.55869   9.68506  L
C-CA--0.234100       0     0.5485   -12.5916   8.52829  L
C-C-0.322600         0     1.82366  -12.69945   9.1191   L
O-OH--0.557900       0     2.4651   -13.89539   9.1245   L
H-H-0.271900         0    -2.62549  -8.04385   10.32801  L
H-H-0.271900         0    -0.04529  -9.9186    11.41295  L
H-H-0.271900         0    -0.45691  -8.54947   12.43676  L
H-H1-0.087600        0     0.90467  -7.65629   10.35627  L
H-HC-0.029500        0     0.08909  -8.29031   8.23822  L
H-HC-0.029500        0    -1.33132  -9.09342   8.93368  L
H-HA-0.169900        0     2.25777  -9.44956   10.06253  L
H-HA-0.169900        0    -1.11247  -11.30166   8.07565  L
H-HA-0.165600        0     3.41627  -11.62796   10.12661  L
H-HA-0.165600        0     0.10064  -13.47168   8.08843  L
H-HO-0.399200        0     3.28653  -13.87688   9.61595  L
H-H1-0.097600        0    -3.33769  -5.27442   10.13467  L
H-H1-0.097600        0    -3.20984  -5.72374   11.84371  L
H-H1-0.097600        0    -4.36845  -6.56955   10.79388  L
N-N--0.415700        0     1.83622  -4.25172   11.90922  L
C-CT--0.059700      -1     2.22302  -3.00239   11.23588  L
C-C-0.597300         0     2.25869  -1.80552   12.20173  L
N-N--0.415700        0     1.25341  -1.6708    13.07432  L
C-CT--0.149000       0     1.14483  -0.59127   14.05591  L
O-O--0.567900        0     3.19381  -1.00802   12.14202  L
C-CT-0.130300        0     1.29586  -2.78287   10.0015  L
C-CT--0.043000       0     1.77014  -3.5083    8.71428  L
C-CT--0.320400       0     1.14274  -1.2978    9.61699  L
C-CT--0.066000       0     2.12253  -4.99767   8.80721  L
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H-H-0.271900          0      0.53362  -2.37726   13.05038  L
H-H-0.271900          0      1.05485  -4.79407   11.53858  L
H-H-0.271900          0      2.3629   -4.59388   12.70254  L
H-H1-0.086900         0      3.24252  -3.11275   10.86977  L
H-HC-0.018700         0      0.29776  -3.14991   10.24841  L
H-HC-0.023600         0      2.64544  -2.99781   8.32659  L
H-HC-0.023600         0      0.9891   -3.41035   7.95948  L
H-HC-0.088200         0      2.12313  -0.85131   9.44614  L
H-HC-0.088200         0      0.62293  -0.74936   10.40289  L
H-HC-0.088200         0      0.55193  -1.20723   8.706    L
H-HC-0.018600         0      2.47768  -5.33774   7.83386  L
H-HC-0.018600         0      1.24213  -5.57674   9.06793  L
H-HC-0.018600         0      2.9117   -5.16612   9.53871  L
H-H1-0.097600         0      0.97935   0.36228   13.55136  L
H-H1-0.097600         0      2.06764  -0.5146    14.63569  L
H-H1-0.097600         0      0.31542  -0.78028   14.73922  L
N-N--0.415700         0      5.07992   1.07196   12.7879  L
C-CT--0.051800       -1      4.48979   2.41488   12.79003  L
C-C-0.597300          0      3.9093    2.74701   14.17252  L
N-N--0.415700         0      4.52052   3.69717   14.88945  L
C-CT--0.149000        0      4.08458   4.12381   16.21895  L
O-O--0.567900         0      2.90984   2.15553   14.56983  L
C-CT-0.110200         0      3.36581   2.51191   11.74351  L
C-CT-0.353100         0      3.82182   2.24663   10.29888  L
C-CT--0.412100        0      2.62425   2.322     9.35581  L
C-CT--0.412100        0      4.88889   3.23537   9.81776  L
H-H-0.271900          0      5.34076   4.13844   14.50402  L
H-H-0.271900          0      4.4586    0.27584   12.63729  L
H-H-0.271900          0      5.97926   0.9102    13.2219  L
H-H1-0.092200         0      5.26068   3.14902   12.55848  L
H-HC-0.045700         0      2.92527   3.5088    11.79498  L
H-HC-0.045700         0      2.58752   1.78867   11.99386  L
H-HC--0.036100        0      4.22394   1.24097   10.23286  L
H-HC-0.100000         0      2.18853   3.32076   9.37475  L
H-HC-0.100000         0      1.87068   1.59916   9.66602  L
H-HC-0.100000         0      2.94452   2.07983   8.34189  L
H-HC-0.100000         0      5.12294   3.03999   8.77442  L
H-HC-0.100000         0      5.80708   3.11186   10.39027  L
H-HC-0.100000         0      4.53058   4.26069   9.917    L
H-H1-0.097600         0      4.73871   4.90998   16.60022  L
H-H1-0.097600         0      4.10835   3.27632   16.9076  L
H-H1-0.097600         0      3.06138   4.50252   16.17215  L
N-N--0.415700         0    -12.41124   0.33841   9.29956  L
C-CT--0.001400       -1    -11.28901   0.00235   10.18501  L
C-C-0.597300          0    -10.40535  -1.11047   9.60407  L
O-O--0.567900         0    -9.20158  -0.94052   9.40081  L
C-CT--0.015200        0    -11.81417  -0.33942   11.5873  L
C-CA--0.001100        0    -12.58003   0.79935   12.23489  L
C-CA--0.190600        0    -11.88112   1.91838   12.7286  L
C-CA--0.190600        0    -13.98696   0.75667   12.31652  L
C-CA--0.234100        0    -12.5866   2.99336   13.30193  L
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C-CA--0.234100       0    -14.695    1.83005   12.89269  L
C-C-0.322600         0    -13.99329   2.95191   13.38641  L
O-OH--0.557900       0    -14.66298   3.99569   13.93939  L
H-H-0.271900         0    -13.16893   0.90342   9.66292  L
H-H-0.271900         0    -12.38658   0.10048   8.31254  L
H-H1-0.087600        0    -10.65461   0.88557   10.2739  L
H-HC-0.029500        0    -10.96615  -0.59065   12.22632  L
H-HC-0.029500        0    -12.45632  -1.21974   11.53132  L
H-HA-0.169900        0    -10.80168   1.95687   12.67169  L
H-HA-0.169900        0    -14.53048  -0.0999    11.94148  L
H-HA-0.165600        0    -12.06784   3.85724   13.69003  L
H-HA-0.165600        0    -15.77219   1.79632   12.95775  L
H-HO-0.399200        0    -15.59955   3.817     14.03536  L
N-N--0.347900        0    -11.05668  -2.23415   9.31077  L
C-CT--0.263700      -1    -10.59198  -3.40498   8.56255  L
C-C-0.734100         0    -11.69333  -3.72955   7.55163  L
O-O--0.589400        0    -12.85132  -3.38907   7.80054  L
C-CT--0.000700       0    -10.22716  -4.51489   9.57325  L
C-CT-0.039000        0    -11.36506  -5.13741   10.40981  L
C-CT-0.048600        0    -12.32454  -6.05421   9.6337   L
N-N2--0.529500       0    -13.14728  -6.8817    10.53693  L
C-CA-0.807600        0    -13.04106  -8.18107   10.75928  L
N-N2--0.862700       0    -12.14982  -8.94229   10.19535  L
N-N2--0.862700       0    -13.86226  -8.76259   11.58842  L
H-H-0.274700         0    -12.05956  -2.19634   9.44412  L
H-H1-0.156000        0    -9.6996   -3.13605   8.00869  L
H-HC-0.032700        0    -9.51541  -4.08068   10.27756  L
H-HC-0.032700        0    -9.67904  -5.30554   9.07441  L
H-HC-0.028500        0    -11.9375  -4.34843   10.89836  L
H-HC-0.028500        0    -10.89304  -5.73624   11.1901  L
H-H1-0.068700        0    -11.75157  -6.68149   8.95929  L
H-H1-0.068700        0    -12.99768  -5.45371   9.02593  L
H-H-0.345600         0    -13.89677  -6.40548   11.00515  L
H-H-0.447800         0    -12.07634  -9.92163   10.36761  L
H-H-0.447800         0    -11.49483  -8.54846   9.50422  L
H-H-0.447800         0    -13.77376  -9.74743   11.75114  L
H-H-0.447800         0    -14.57662  -8.2337    12.05315  L
N-N--0.415700        0    -11.35062  -4.31564   6.41659  L
C-CT--0.003100      -1    -12.28129  -4.54386   5.30985  L
C-C-0.597300         0    -13.16683  -5.80085   5.47476  L
N-N--0.415700        0    -12.77042  -6.77363   6.30544  L
C-CT--0.149000      -1    -13.53208  -7.98674   6.60739  L
O-O--0.567900        0    -14.22503  -5.8814    4.85074  L
C-CT--0.003600       0    -11.51422  -4.57977   3.97809  L
C-CT--0.064500       0    -10.99753  -3.17511   3.63614  L
C-C-0.695100         0    -10.3495  -3.06977   2.26168  L
O-O--0.608600        0    -9.63489  -3.94882   1.79134  L
N-N--0.940700        0    -10.54106  -1.95679   1.59384  L
H-H-0.271900         0    -10.44183  -4.76098   6.40523  L
H-H-0.271900         0    -11.82061  -6.69259   6.66584  L
H-H1-0.085000        0    -12.97749  -3.70363   5.26445  L
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H-HC-0.017100        0    -12.18855  -4.9031    3.18365  L
H-HC-0.017100        0    -10.68278  -5.28273   4.04597  L
H-HC-0.035200        0    -10.26265  -2.86547   4.37864  L
H-HC-0.035200        0    -11.83476  -2.47702   3.67887  L
H-H-0.425100         0    -9.77068  -1.72594   0.97458  L
H-H-0.425100         0    -11.12205  -1.23576   1.99732  L
H-H1-0.097600        0    -12.93885  -8.63593   7.25281  L
H-H1-0.097600        0    -13.75001  -8.51477   5.67796  L
H-H1-0.097600        0    -14.46887  -7.72331   7.09954  L
N-N--0.347900        0    -14.84154  -14.79719  -4.35865  L
C-CT--0.240000       -1   -14.79913  -13.32623  -4.37238  L
C-C-0.734100         0    -15.53456  -12.75171  -5.61232  L
N-N-0.415700         0    -15.93776  -11.47753  -5.68295  L
C-CT-0.149000        0    -15.89129  -10.44235  -4.659    L
O-O--0.589400        0    -15.73431  -13.48298  -6.57063  L
C-CT--0.009400       0    -13.31127  -12.86665  -4.38396  L
C-CT-0.018700        0    -12.44795  -13.22664  -3.15027  L
C-CT--0.047900       0    -11.05799  -12.54195  -3.19083  L
C-CT--0.014300       0    -10.09731  -13.06929  -2.10507  L
N-N3--0.385400       0    -8.79906  -12.34172  -2.07604  L
H-H-0.274700         0    -16.35698  -11.26611  -6.57592  L
H-H-0.271900         0    -14.60325  -15.33223  -3.52939  L
H-H-0.271900         0    -15.06612  -15.30042  -5.21571  L
H-H1-0.142600        0    -15.27987  -12.97056  -3.45885  L
H-HC-0.036200        0    -13.28918  -11.78576  -4.48928  L
H-HC-0.036200        0    -12.82519  -13.28154  -5.27015  L
H-HC-0.010300        0    -12.31204  -14.30855  -3.11849  L
H-HC-0.010300        0    -12.96692  -12.91354  -2.24317  L
H-HC-0.062100        0    -11.18761  -11.46635  -3.05759  L
H-HC-0.062100        0    -10.60252  -12.71661  -4.16747  L
H-HP-0.113500        0    -9.90965  -14.13058  -2.29058  L
H-HP-0.113500        0    -10.57529  -12.97772  -1.12476  L
H-H-0.340000         0    -8.36299  -12.23185  -2.98101  L
H-H-0.340000         0    -8.08601  -12.82493  -1.52357  L
H-H-0.340000         0    -8.86952  -11.40683  -1.66734  L
H-H1-0.097600        0    -15.4478  -10.81151  -3.73548  L
H-H1-0.097600        0    -16.90272  -10.09501  -4.44116  L
H-H1-0.097600        0    -15.30457  -9.59679  -5.01996  L
N-N--0.254800        0    -15.66767  -9.14187  -1.49853  L
C-CT--0.026600       -1   -14.71612  -8.08569  -1.82167  L
C-C-0.589600         0    -13.5653  -8.58619  -2.70292  L
O-O--0.574800        0    -13.33018  -9.7862   -2.86283  L
C-CT--0.007000       0    -14.23076  -7.5474   -0.46704  L
C-CT-0.018900        0    -14.46351  -8.70613   0.50495  L
C-CT-0.019200        0    -15.71188  -9.37801  -0.06677  L
H-H1-0.064100        0    -15.23653  -7.28664  -2.35113  L
H-HC-0.025300        0    -14.85443  -6.70168  -0.17126  L
H-HC-0.025300        0    -13.18286  -7.24655  -0.48856  L
H-HC-0.021300        0    -14.62739  -8.35107   1.52338  L
H-HC-0.215300        0    -13.62113  -9.39928   0.4767   L
H-H1-0.039100        0    -15.71225  -10.44528   0.15757  L
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H-H1-0.039100        0    -16.60593  -8.90883   0.34753  L
N-N--0.415700        0    -12.88721  -7.64356  -3.34539  L
C-CT--0.038900       -1   -11.66891  -7.76914  -4.16743  L
C-C-0.597300         0    -11.0807  -6.36355  -4.1755   L
O-O--0.567900        0    -11.84456  -5.40837  -4.329    L
C-CT-0.365400        0    -11.99715  -8.24755  -5.59434  L
O-OH--0.676100       0    -12.79032  -9.41951  -5.51572  L
C-CT--0.243800       0    -10.73764  -8.6072   -6.37644  L
H-H-0.271900         0    -13.17517  -6.68442  -3.192    L
H-H1-0.100700        0    -10.96237  -8.45547  -3.69612  L
H-H1-0.004300        0    -12.5528  -7.47583  -6.12873  L
H-HC-0.064200        0    -10.10486  -7.72746  -6.49503  L
H-HC-0.064200        0    -11.0143  -8.97391  -7.36522  L
H-HC-0.064200        0    -10.17666  -9.38111  -5.85122  L
H-HO-0.410200        0    -12.64751  -9.73504  -4.60934  L
N-N--0.415700        0    -9.78539  -6.21543  -3.91793  L
C-CT--0.001400       -1   -9.12575  -4.94013  -3.60794  L
C-C-0.597300         0    -9.53764  -3.78461  -4.53126  L
O-O--0.567900        0    -10.04063  -2.78837  -4.02709  L
C-CT--0.015200       0    -7.63018  -5.19011  -3.59472  L
C-CA--0.001100       0    -6.79488  -3.93873  -3.75294  L
C-CA--0.190600       0    -6.22592  -3.65372  -5.00754  L
C-CA--0.190600       0    -6.68253  -3.01344  -2.6981   L
C-CA--0.234100       0    -5.59872  -2.42033  -5.22999  L
C-CA--0.234100       0    -6.06412  -1.76969  -2.92266  L
C-C-0.322600         0    -5.56193  -1.45752  -4.20301  L
O-OH--0.557900       0    -5.09685  -0.21637  -4.48614  L
H-H-0.271900         0    -9.21999  -7.06032  -3.81519  L
H-H1-0.087600        0    -9.4063   -4.64089  -2.59705  L
H-HC-0.029500        0    -7.37302  -5.88745  -4.39257  L
H-HC-0.029500        0    -7.43635  -5.66873  -2.64119  L
H-HA-0.169900        0    -6.3099   -4.35938  -5.82186  L
H-HA-0.169900        0    -7.11255  -3.22272  -1.72448  L
H-HA-0.165600        0    -5.17121  -2.18587  -6.19231  L
H-HA-0.165600        0    -6.02788  -1.04185  -2.12327  L
H-HO-0.399200        0    -4.89085   0.28623  -3.67049  L
N-N--0.415700        0    -9.43523  -3.94646  -5.85875  L
C-CT-0.014300        -1   -9.85408  -2.97959  -6.89407  L
C-C-0.597300         0    -11.29719  -2.45136  -6.8092   L
O-O--0.567900        0    -11.63958  -1.52545  -7.53382  L
C-CT--0.204100       0    -9.56609  -3.58811  -8.28136  L
C-C-0.713000         0    -8.10032  -3.50712  -8.66857  L
O-O--0.593100        0    -7.26479  -4.27702  -8.22367  L
N-N--0.919100        0    -7.73533  -2.5715   -9.51119  L
H-H-0.271900         0    -8.95392  -4.77848  -6.16644  L
H-H1-0.104800        0    -9.23011  -2.09133  -6.7834   L
H-HC-0.079700        0    -10.14267  -3.05173  -9.03645  L
H-HC-0.079700        0    -9.88376  -4.62948  -8.30925  L
H-H-0.419600         0    -6.7917   -2.626    -9.84741  L
H-H-0.419600         0    -8.44888  -1.97493  -9.93145  L
N-N--0.415700        0    -12.1206  -3.00502  -5.92314  L
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C-CT--0.002400       -1   -13.42793  -2.48533  -5.54724  L
C-C-0.597300         0    -13.51026  -2.10491  -4.06799  L
O-O--0.567900        0    -13.9839  -1.02316  -3.73522  L
C-CT--0.034300       0    -14.49943  -3.518    -5.92358  L
C-CA-0.011800        0    -15.91072  -3.09     -5.56913  L
C-CA--0.125600       0    -16.61743  -2.22451  -6.42491  L
C-CA--0.125600       0    -16.50756  -3.52725  -4.36975  L
C-CA--0.170400       0    -17.9163  -1.80481  -6.08763  L
C-CA--0.170400       0    -17.80721  -3.10763  -4.03382  L
C-CA--0.107200       0    -18.5115  -2.24668  -4.89345  L
H-H-0.271900         0    -11.73463  -3.75574  -5.36822  L
H-H1-0.097800        0    -13.635   -1.57352  -6.11222  L
H-HC-0.029500        0    -14.28034  -4.46277  -5.42443  L
H-HC-0.029500        0    -14.45064  -3.6957   -6.99914  L
H-HA-0.133000        0    -16.16185  -1.86651  -7.33804  L
H-HA-0.133000        0    -15.96533  -4.16781  -3.69191  L
H-HA-0.143000        0    -18.45392  -1.13103  -6.74131  L
H-HA-0.143000        0    -18.26414  -3.42667  -3.10769  L
H-HA-0.129700        0    -19.50596  -1.91089  -4.63183  L
N-N--0.415700        0    -13.04255  -2.98293  -3.17713  L
C-CT-0.033700        -1   -13.00925  -2.74014  -1.73685  L
C-C-0.597300         0    -12.34443  -1.39878  -1.38203  L
O-O--0.567900        0    -12.93053  -0.58676  -0.66949  L
C-CT--0.182500       0    -12.32545  -3.93015  -1.05008  L
H-H-0.271900         0    -12.60557  -3.81898  -3.53902  L
H-H1-0.082300        0    -14.03764  -2.68272  -1.37579  L
H-HC-0.060300        0    -12.84435  -4.85383  -1.30068  L
H-HC-0.060300        0    -12.35622  -3.78842   0.03158  L
H-HC-0.060300        0    -11.28322  -3.99881  -1.36265  L
N-N--0.415700        0    -11.15398  -1.15032  -1.93734  L
C-CT--0.087500       -1   -10.42655   0.11781  -1.81566  L
C-C-0.597300         0    -11.24687   1.31837  -2.26887  L
O-O--0.567900        0    -11.16907   2.3675   -1.6501   L
C-CT-0.298500        0    -9.06568   0.03958  -2.54087  L
C-CT--0.319200       0    -9.13389   0.24189  -4.06005  L
C-CT--0.319200       0    -8.06062   1.04911  -1.98356  L
H-H-0.271900         0    -10.75793  -1.85987  -2.54397  L
H-H1-0.096900        0    -10.22078   0.26774  -0.7551   L
H-HC--0.029700       0    -8.65721  -0.9531   -2.35744  L
H-HC-0.079100        0    -8.18712  -0.07009  -4.49485  L
H-HC-0.079100        0    -9.30873   1.2924   -4.29826  L
H-HC-0.079100        0    -9.93041  -0.35757  -4.49233  L
H-HC-0.079100        0    -7.80992   0.77871  -0.96019  L
H-HC-0.079100        0    -8.48233   2.05354  -2.00893  L
H-HC-0.079100        0    -7.14682   1.0333   -2.57502  L
N-N--0.415700        0    -12.03374   1.17174  -3.33637  L
C-CT--0.087500       -1   -12.82796   2.25122  -3.92976  L
C-C-0.597300         0    -13.96053   2.69026  -3.01132  L
O-O--0.567900        0    -14.12686   3.88186  -2.76506  L
C-CT-0.298500        0    -13.35768   1.8843   -5.3324   L
C-CT--0.319200       0    -14.04072   3.07925  -6.00873  L
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C-CT--0.319200       0    -12.21581   1.43133  -6.25074  L
H-H-0.271900         0    -12.11132   0.24788  -3.73146  L
H-H1-0.096900        0    -12.17446   3.1171   -4.04523  L
H-HC--0.029700       0    -14.08117   1.07409  -5.254    L
H-HC-0.079100        0    -14.3589    2.80404  -7.01527  L
H-HC-0.079100        0    -13.34823   3.91902  -6.07693  L
H-HC-0.079100        0    -14.92084   3.38517  -5.44347  L
H-HC-0.079100        0    -11.74952   0.52962  -5.86225  L
H-HC-0.079100        0    -11.47026   2.22196  -6.33283  L
H-HC-0.079100        0    -12.61003   1.20633  -7.24233  L
N-N--0.415700        0    -14.72883   1.73185  -2.48961  L
C-CT--0.087500       -1   -15.76369   1.99081  -1.47774  L
C-C-0.597300         0    -15.1668    2.69243  -0.26397  L
O-O--0.567900        0    -15.63218   3.75323   0.14108  L
C-CT-0.298500        0    -16.49319   0.68952  -1.0818   L
C-CT--0.319200       0    -17.57372   0.93744  -0.02052  L
C-CT--0.319200       0    -17.18332   0.04826  -2.29471  L
H-H-0.271900         0    -14.51163   0.77686  -2.75228  L
H-H1-0.096900        0    -16.4973    2.67371  -1.90618  L
H-HC--0.029700       0    -15.77186  -0.0237   -0.68131  L
H-HC-0.079100        0    -18.09842   0.00819   0.20084  L
H-HC-0.079100        0    -18.28868   1.67854  -0.37948  L
H-HC-0.079100        0    -17.12003   1.29675   0.90346  L
H-HC-0.079100        0    -17.89481   0.74798  -2.73398  L
H-HC-0.079100        0    -17.71079  -0.85361  -1.98659  L
H-HC-0.079100        0    -16.44849  -0.23011  -3.04926  L
N-N--0.516300        0    -14.14053   2.08626   0.31786  L
C-CT-0.038100        -1   -13.52584   2.48964   1.57831  L
C-C-0.536600         0    -12.70159   3.78296   1.47501  L
O-O--0.581900        0    -12.62139   4.5397    2.43476  L
C-CT--0.030300       0    -12.71868   1.26944   2.04674  L
C-C-0.799400         0    -12.54665   1.19932   3.55687  L
O-O2--0.801400       0    -12.17708   2.23101   4.15327  L
O-O2--0.801400       0    -12.66804   0.08085   4.10156  L
H-H-0.293600         0    -13.7992    1.22982  -0.1054   L
H-H1-0.088000        0    -14.31968   2.66938   2.30481  L
H-HC--0.012200       0    -11.74631   1.25793   1.55341  L
H-HC--0.012200       0    -13.24591   0.36004   1.75103  L
N-N--0.516300        0    -12.12538   4.11028   0.31722  L
C-CT-0.038100        -1   -11.48413   5.4129    0.10495  L
C-C-0.536600         0    -12.45479   6.59376  -0.02778  L
O-O--0.581900        0    -12.02038   7.74034   0.08274  L
C-CT--0.030300       0    -10.4252    5.37046  -1.01972  L
C-C-0.799400         0    -9.10428    4.70515  -0.58748  L
O-O2--0.801400       0    -8.92892    4.371     0.60727  L
O-O2--0.801400       0    -8.16414    4.59131  -1.40893  L
H-H-0.293600         0    -12.14232   3.44676  -0.45118  L
H-H1-0.088000        0    -10.93509   5.64934   1.01665  L
H-HC--0.012200       0    -10.18254   6.39482  -1.30675  L
H-HC--0.012200       0    -10.83428   4.87855  -1.90202  L
N-N--0.415700        0    -13.76183   6.3471   -0.14845  L
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C-CT--0.058100       -1   -14.79691   7.38687  -0.14519  L
C-C-0.597300         0    -15.75604   7.21273   1.03834  L
N-N--0.415700        0    -16.65528   6.22773   0.99251  L
C-CT--0.149000       0    -17.62538   5.91947   2.03991  L
O-O--0.567900        0    -15.65071   7.95029   2.0211   L
C-CT--0.007400       0    -15.47996   7.44936  -1.51697  L
C-CC-0.186800        0    -14.54216   7.97451  -2.57498  L
N-NB--0.543200       0    -14.12563   9.30139  -2.68688  L
C-CW--0.220700       0    -13.9024   7.22427  -3.51679  L
C-CR-0.163500        0    -13.24906   9.32268  -3.70129  L
N-NA--0.279500       0    -13.09406   8.09084  -4.22033  L
H-H-0.271900         0    -14.03496   5.37363  -0.22726  L
H-H-0.271900         0    -16.54118   5.55634   0.23978  L
H-H1-0.136000        0    -14.33038   8.36113   0.0035   L
H-HC-0.036700        0    -16.33608   8.12228  -1.45991  L
H-HC-0.036700        0    -15.8356   6.45796  -1.8024   L
H-H4-0.186200        0    -14.00029   6.15597  -3.6495   L
H-H-0.333900         0    -12.47819   7.84796  -4.98415  L
H-H5-0.143500        0    -12.73702   10.2106  -4.0471   L
H-H1-0.097600        0    -18.10247   6.83668   2.39019  L
H-H1-0.097600        0    -17.12066   5.43265   2.87568  L
H-H1-0.097600        0    -18.38867   5.24621   1.64679  L
N-N--0.415700        0    -13.98956   6.36434   3.93976  L
C-CT--0.023700       -1   -13.16025   7.04403   4.93479  L
C-C-0.597300         0    -12.97457   8.56264   4.68501  L
N-N--0.415700        0    -13.67364   9.1496    3.70793  L
C-CT--0.149000       0    -13.77056   10.58841   3.4768   L
O-O--0.567800        0    -12.2413   9.23325   5.42529  L
C-CT-0.034200        0    -11.80989   6.33199   5.12315  L
C-CT-0.001800        0    -11.96768   5.02817   5.90531  L
S-S--0.273700        0    -10.39469   4.33355   6.48049  L
C-CT--0.053600       0    -11.02135   2.85503   7.31949  L
H-H-0.271900         0    -14.25891   8.5562    3.12495  L
H-H-0.271900         0    -13.60267   5.53435   3.48963  L
H-H-0.271900         0    -14.80663   6.80214   3.52516  L
H-H1-0.088000        0    -13.691    6.97905   5.88439  L
H-HC-0.024100        0    -11.15123   6.97093   5.70914  L
H-HC-0.024100        0    -11.33778   6.14015   4.15863  L
H-H1-0.044000        0    -12.48339   4.30443   5.27839  L
H-H1-0.044000        0    -12.58821   5.21469   6.78162  L
H-H1-0.068400        0    -11.67534   3.14997   8.13933  L
H-H1-0.068400        0    -10.18517   2.27632   7.71117  L
H-H1-0.068400        0    -11.58481   2.24473   6.61251  L
H-H1-0.097600        0    -12.77742   11.03575   3.46092  L
H-H1-0.097600        0    -14.36846   11.04894   4.26494  L
H-H1-0.097600        0    -14.26093   10.76617   2.51702  L
N-N--0.415700        0    -11.69983   10.3576   1.03133  L
C-CT--0.059700       -1   -10.33642   10.78338   1.35585  L
C-C-0.597300         0    -9.98217   11.98019   0.45016  L
N-N--0.415700        0    -10.10286   13.19673   0.99509  L
C-CT--0.149000       0    -9.83552   14.46435   0.31435  L
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O-O--0.567900        0    -9.63068   11.82042  -0.71793  L
C-CT-0.130300        0    -9.37206   9.58295   1.17294  L
C-CT--0.043000       0    -9.61238   8.47451   2.22838  L
C-CT--0.320400       0    -7.88384   9.97551   1.15509  L
C-CT--0.066000       0    -9.32918   8.85833   3.68844  L
H-H-0.271900         0    -10.42264   13.23098   1.94668  L
H-H-0.271900         0    -11.84279   9.35239   0.91568  L
H-H-0.271900         0    -12.22955   10.92959   0.3848   L
H-H1-0.086900        0    -10.29456   11.1189   2.38881  L
H-HC-0.018700        0    -9.58255   9.14487   0.19487  L
H-HC-0.023600        0    -8.99541   7.61256   1.97238  L
H-HC-0.023600        0    -10.64805   8.14323   2.17586  L
H-HC-0.088200        0    -7.29088   9.10858   0.87869  L
H-HC-0.088200        0    -7.5624    10.36429   2.11803  L
H-HC-0.088200        0    -7.68712   10.7282   0.39858  L
H-HC-0.018600        0    -9.96786   9.68219   4.00143  L
H-HC-0.018600        0    -8.28671   9.13462   3.82382  L
H-HC-0.018600        0    -9.53547   7.99784   4.31983  L
H-H1-0.097600        0    -10.55381   15.2208   0.63409  L
H-H1-0.097600        0    -9.92456   14.34136  -0.76799  L
H-H1-0.097600        0    -8.82604   14.80729   0.54796  L
N-N--0.415703        0    -7.0439    13.0849  -0.94029  L
C-CT--0.058100       -1   -5.66114   12.76253  -1.28607  L
C-C-0.597300         0    -5.41293   11.25178  -1.23486  L
O-O--0.567900        0    -4.92298   10.69316  -0.24786  L
C-CT--0.007400       0    -4.73281   13.54004  -0.33333  L
C-CC-0.186800        0    -5.00109   15.02499  -0.27198  L
N-NB--0.543200       0    -5.9835    15.6419   0.51198  L
C-CW--0.220700       0    -4.33038   15.97674  -0.98063  L
C-CR-0.163500        0    -5.88061   16.95466   0.25029  L
N-NA--0.279500       0    -4.8976    17.18544  -0.6387   L
H-H-0.271900         0    -7.16582   13.77889  -0.20891  L
H-H-0.271900         0    -7.8243    12.46692  -1.15688  L
H-H1-0.136000        0    -5.45827   13.10892  -2.29962  L
H-HC-0.036700        0    -3.69628   13.3777  -0.6273   L
H-HC-0.036700        0    -4.85303   13.15269   0.6728   L
H-H4-0.186200        0    -3.51445   15.80251  -1.66857  L
H-H-0.333900         0    -4.6285    18.09638  -0.98813  L
H-H5-0.143500        0    -6.5023    17.72333   0.69146  L
N-N--0.415700        0    -5.77993   10.57273  -2.3224   L
C-CT--0.087500       -1   -5.72976   9.10789  -2.43821  L
C-C-0.597300         0    -4.30832   8.65407  -2.78138  L
O-O--0.567900        0    -3.99279   8.23429  -3.89311  L
C-CT-0.298500        0    -6.7989    8.59789  -3.43408  L
C-CT--0.319200       0    -7.00214   7.09107  -3.26921  L
C-CT--0.319200       0    -8.17318   9.24783  -3.19931  L
H-H-0.271900         0    -6.22147   11.08747  -3.06963  L
H-H1-0.096900        0    -5.98806   8.6906   -1.47098  L
H-HC--0.029700       0    -6.49124   8.82196  -4.45382  L
H-HC-0.079100        0    -6.07102   6.55254  -3.43984  L
H-HC-0.079100        0    -7.74447   6.73802  -3.98534  L
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 H-HC-0.079100        0    -7.37672   6.87987  -2.27017  L
 H-HC-0.079100        0    -8.49159   9.10481  -2.16593  L
 H-HC-0.079100        0    -8.91173   8.79042  -3.85983  L
 H-HC-0.079100        0    -8.14572   10.31236  -3.426    L
 N-N--0.415700        0    -3.41027   8.84216  -1.82022  L
 C-CT--0.002400       -1   -1.97074   8.71559  -2.01091  L
 C-C-0.597300         0    -1.48081   7.30057  -1.68045  L
 O-O--0.567900        0    -1.99008   6.64549  -0.76459  L
 C-CT--0.034300       0    -1.24486   9.76271  -1.15274  L
 C-CA-0.011800        0    -1.32502   11.22371  -1.58375  L
 C-CA--0.125600       0    -2.1655    11.67559  -2.62652  L
 C-CA--0.125600       0    -0.48354   12.14868  -0.93701  L
 C-CA--0.170400       0    -2.15345   13.02667  -3.01779  L
 C-CA--0.170400       0    -0.47692   13.5007  -1.32144  L
 C-CA--0.107200       0    -1.30617   13.93914  -2.36708  L
 H-H-0.271900         0    -3.74303   9.26325  -0.96195  L
 H-H1-0.097800        0    -1.72224   8.90843  -3.05549  L
 H-HC-0.029500        0    -0.18572   9.49999  -1.14079  L
 H-HC-0.029500        0    -1.60713   9.68542  -0.12718  L
 H-HA-0.133000        0    -2.79819   10.99855  -3.17455  L
 H-HA-0.133000        0     0.18285   11.81457  -0.15203  L
 H-HA-0.143000        0    -2.76411   13.35876  -3.84647  L
 H-HA-0.143000        0     0.1908    14.19581  -0.83053  L
 H-HA-0.129700        0    -1.26923   14.97171  -2.68561  L
 N-N--0.347900        0    -0.49191   6.82968  -2.44638  L
 C-CT--0.263700       -1    0.12801   5.49819  -2.37279  L
 C-C-0.734100         0     1.38362   5.40066  -3.23866  L
 O-O--0.589400        0     1.8791    6.42553  -3.69416  L
 C-CT--0.000700       0    -0.91204   4.43832  -2.79043  L
 C-CT-0.039000        0    -1.51493   4.61541  -4.19036  L    H-H1
1046  0.        0.
 C-CT-0.048600        0    -2.63752   3.59361  -4.34181  H
 N-N2--0.529500       0    -3.30472   3.74502  -5.62693  H
 C-CA-0.807600        0    -4.55745   3.34469  -5.81181  H
 N-N2--0.862700       0    -5.25181   2.81548  -4.81363  H
 N-N2--0.862700       0    -5.11909   3.45519  -7.03292  H
 H-H-0.274700         0    -0.18185   7.41596  -3.21914  L
 H-H1-0.156000        0     0.43214   5.29469  -1.346    L
 H-HC-0.032700        0    -1.71658   4.45774  -2.06422  L
 H-HC-0.032700        0    -0.47331   3.44443  -2.73648  L
 H-HC-0.028500        0    -0.7523    4.44992  -4.95211  L
 H-HC-0.028500        0    -1.93129   5.61724  -4.30319  L
 H-H1-0.068700        0    -3.36907   3.76952  -3.54931  H
 H-H1-0.068700        0    -2.24238   2.58256  -4.21171  H
 H-H-0.345600         0    -2.76285   3.9139   -6.46195  H
 H-H-0.447800         0    -6.21685   2.57105  -5.04814  H
 H-H-0.447800         0    -4.82826   2.35567  -3.99033  H
 H-H-0.447800         0    -6.10096   3.18598  -7.07593  H
 H-H-0.447800         0    -4.83256   4.17308  -7.68901  H
 N-N--0.415700        0     1.88748   4.1899   -3.47494  L
 C-CT--0.025200       -1    3.03708   3.91208  -4.33345  L
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 C-C-0.597300          0     2.70077   3.74553  -5.81645  L
 O-O--0.567900         0     1.56343   3.50688  -6.22912  L
 H-H-0.271900          0     1.40923   3.38543  -3.08313  L
 H-H1-0.069800         0     3.50087   2.98443  -3.9986   L
 H-H1-0.069800         0     3.76497   4.71239  -4.2171   L
 N-N--0.516300         0     3.75182   3.8541   -6.61919  L
 C-CT-0.039700         0     3.83674   3.58761  -8.05828  L
 C-C-0.536600          0     3.32216   2.18991  -8.44232  L
 O-O--0.581900         0     2.69876   2.02441  -9.49064  L
 C-CT-0.056000         0     5.30306   3.81409  -8.43431  L
 C-CT-0.013600         0     5.683     3.58817  -9.8978   L
 C-C-0.805400          0     7.11949   4.07838  -10.12706  L
 O-O2--0.818800        0     8.04742   3.60687  -9.42925  L
 O-O2--0.818800        0     7.33565   4.978    -10.96593  L
 H-H-0.293600          0     4.60996   4.16082  -6.16965  L
 H-H1-0.110500         0     3.23733   4.31796  -8.60023  L
 H-HC--0.017300        0     5.9307    3.17837  -7.80691  L
 H-HC--0.017300        0     5.52208   4.85412  -8.19806  L
 H-HC--0.042500        0     4.98889   4.13908  -10.5369  L
 H-HC--0.042500        0     5.61118   2.52451  -10.13468  L
 N-N--0.516300         0     3.49621   1.19656  -7.56302  L
 C-CT-0.038100        -1     2.95379  -0.1626   -7.69677  L
 C-C-0.536600          0     1.41938  -0.22526  -7.87618  L
 O-O--0.581900         0     0.90532  -1.24454  -8.34609  L
 C-CT--0.030300        0     3.44627  -1.04469  -6.53237  L
 C-C-0.799400          0     2.78304  -0.80723  -5.17287  L
 O-O2--0.801400        0     2.55468   0.35957  -4.78896  L
 O-O2--0.801400        0     2.56426  -1.81911  -4.46069  L
 H-H-0.293600          0     3.92051   1.43798  -6.67839  L
 H-H1-0.088000         0     3.37944  -0.58069  -8.60936  L
 H-HC--0.012200        0     4.51744  -0.91313  -6.40565  L
 H-HC--0.012200        0     3.2954   -2.08538  -6.81337  L
 N-N--0.415700         0     0.69874   0.86403  -7.57229  L
 C-CT--0.058100        0    -0.74614   1.03529  -7.78089  L    H-HC
1102  0.        0.
 C-C-0.597300          0    -1.12438   2.23719  -8.67479  L
 O-O--0.567900         0    -2.30308   2.59498  -8.76545  L
 C-CT--0.007400        0    -1.42916   1.08248  -6.40711  H
 C-CC-0.186800         0    -1.49576  -0.24358  -5.71975  H
 N-NB--0.543200        0    -2.46532  -1.15296  -6.07915  H
 C-CW--0.220700        0    -0.68193  -0.77627  -4.75543  H
 C-CR-0.163500         0    -2.23901  -2.21044  -5.33146  H
 N-NA--0.279500        0    -1.16621  -2.03643  -4.52315  H
 H-H-0.271900          0     1.21429   1.61763  -7.1257   L
 H-H1-0.136000         0    -1.12909   0.15614  -8.29876  L
 H-HC-0.036700         0    -2.4633    1.41469  -6.54618  H
 H-HC-0.036700         0    -0.90306   1.82165  -5.79287  H
 H-H4-0.186200         0     0.17727  -0.39212  -4.2291   H
 H-H-0.333900          0    -0.81333  -2.69401  -3.83126  H
 H-H5-0.143500         0    -2.81254  -3.12767  -5.32815  H
 N-N--0.415700         0    -0.17732   2.81305  -9.42704  L
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C-CT--0.051800       -1   -0.46583   3.68511  -10.58189  L
C-C-0.597300         0    -1.33701   2.93279  -11.59392  L
O-O--0.567900        0    -2.46524   3.32474  -11.88039  L
C-CT--0.110200       0     0.86607   4.16968  -11.19275  L
C-CT-0.353100        0     0.73034   5.01067  -12.47686  L
C-CT--0.412100       0    -0.07164   6.29353  -12.26682  L
C-CT--0.412100       0     2.12093   5.39315  -12.98065  L
H-H-0.271900         0     0.77899   2.48893  -9.29904  L
H-H1-0.092200        0    -1.03079   4.55232  -10.24523  L
H-HC-0.045700        0     1.48056   3.30043  -11.42932  L
H-HC-0.045700        0     1.40296   4.75491  -10.4474  L
H-HC--0.036100       0     0.24118   4.41468  -13.24747  L
H-HC-0.100000        0    -1.08932   6.06389  -11.9557  L
H-HC-0.100000        0    -0.11542   6.85643  -13.19909  L
H-HC-0.100000        0     0.40839   6.91098  -11.50734  L
H-HC-0.100000        0     2.63511   6.00544  -12.23818  L
H-HC-0.100000        0     2.03725   5.95719  -13.90973  L
H-HC-0.100000        0     2.71068   4.49576  -13.16835  L
N-N--0.415700        0    -0.83035   1.79359  -12.06051  L
C-CT--0.024900       -1   -1.47618   0.83435  -12.9636  L
C-C-0.597300         0    -2.93479   0.49781  -12.60484  L
O-O--0.567900        0    -3.77352   0.40321  -13.5028  L
C-CT-0.211700        0    -0.63292  -0.44752  -12.97344  L
O-OH--0.654600       0    -0.5463   -0.95498  -11.65308  L
H-H-0.271900         0     0.07759   1.5452   -11.69119  L
H-H1-0.084300        0    -1.4739    1.25525  -13.96909  L
H-H1-0.035200        0     0.36866  -0.21651  -13.34052  L
H-H1-0.035200        0    -1.09058  -1.19107  -13.62766  L
H-HO-0.427500        0     0.23112  -1.51976  -11.56388  L
N-N--0.415700        0    -3.24213   0.28275  -11.3197  L
C-CT-0.014300        -1   -4.57882  -0.0417   -10.79551  L
C-C-0.597300         0    -5.54613   1.1441   -10.79155  L
O-O--0.567900        0    -6.75083   0.91528  -10.80707  L
C-CT--0.204100       0    -4.4294   -0.697    -9.41974  L
C-C-0.713000         0    -3.74052  -2.04001  -9.54281  L
O-O--0.593100        0    -4.09115  -2.85973  -10.38489  L
N-N--0.919100        0    -2.75994  -2.30915  -8.72582  L
H-H-0.271900         0    -2.45343   0.29838  -10.6873  L
H-H1-0.104800        0    -5.03296  -0.77402  -11.46521  L
H-HC-0.079700        0    -5.41801  -0.87796  -9.00918  L
H-HC-0.079700        0    -3.88056  -0.04129  -8.74196  L
H-H-0.419600         0    -2.36936  -3.24489  -8.75244  L
H-H-0.419600         0    -2.52845  -1.70478  -7.94282  L
N-N--0.415700        0    -5.0477    2.38285  -10.82115  L
C-CT--0.038900       -1   -5.85479   3.6159   -10.78723  L
C-C-0.597300         0    -6.98806   3.63874  -11.81396  L
O-O--0.567900        0    -8.14014   3.70911  -11.40099  L
C-CT-0.365400        0    -4.98187   4.86996  -10.72154  L
O-OH--0.676100       0    -4.1978    4.74044  -9.54928  L
C-CT--0.243800       0    -5.78986   6.15281  -10.57406  L
H-H-0.271900         0    -4.0411    2.47564  -10.89339  L
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H-H1-0.100700        0    -6.37645   3.59794  -9.82963  L
H-H1-0.004300        0    -4.34134   4.94689  -11.59813  L
H-HC-0.064200        0    -5.1195    6.99795  -10.42077  L
H-HC-0.064200        0    -6.46155   6.07128  -9.71984  L
H-HC-0.064200        0    -6.3794    6.33433  -11.4724  L
H-HO-0.410200        0    -3.52141   4.06705  -9.72596  L
N-N--0.254800        0    -6.75599   3.46688  -13.12371  L
C-CT--0.026600       -1   -7.85299   3.39521  -14.09292  L
C-C-0.589600         0    -8.60034   2.04661  -14.17642  L
O-O--0.574800        0    -9.38069   1.83964  -15.09884  L
C-CT--0.007000       0    -7.17417   3.73836  -15.42856  L
C-CT-0.018900        0    -5.76445   3.17361  -15.26116  L
C-CT-0.019200        0    -5.4646    3.48471  -13.79757  L
H-H1-0.064100        0    -8.59477   4.16632  -13.87854  L
H-HC-0.025300        0    -7.11799   4.82312  -15.53638  L
H-HC-0.025300        0    -7.68131   3.30899  -16.29343  L
H-HC-0.021300        0    -5.05127   3.65429  -15.93161  L
H-HC-0.021300        0    -5.7764    2.09361  -15.41578  L
H-H1-0.039100        0    -4.7788    2.74514  -13.39011  L
H-H1-0.039100        0    -5.02888   4.48188  -13.72163  L
N-N--0.347900        0    -8.42301   1.13602  -13.21095  L
C-CT--0.240000       -1   -9.36594   0.03275  -12.92017  L
C-C-0.734100         0    -9.70426   0.05706  -11.41252  L
O-O--0.589400        0    -9.80064  -0.97833  -10.75277  L
C-CT--0.009400       0    -8.82079  -1.35182  -13.33928  L
C-CT-0.018700        0    -8.05963  -1.44572  -14.67166  L
C-CT--0.047900       0    -6.55325  -1.2533   -14.44923  L
C-CT--0.014300       0    -5.76323  -1.54684  -15.72423  L
N-N3--0.385400       0    -4.31334  -1.5512   -15.42618  L
H-H-0.274700         0    -7.75938   1.37081  -12.47992  L
H-H1-0.142600        0    -10.30036   0.20512  -13.45978  L
H-HC-0.036200        0    -9.67857  -2.02405  -13.40012  L
H-HC-0.036200        0    -8.17778  -1.74187  -12.54861  L
H-HC-0.010300        0    -8.44258  -0.71945  -15.38908  L
H-HC-0.010300        0    -8.2165   -2.44528  -15.08002  L
H-HC-0.062100        0    -6.22325  -1.94033  -13.66752  L
H-HC-0.062100        0    -6.35276  -0.23247  -14.12415  L
H-HP-0.113500        0    -6.00396  -0.78555  -16.47277  L
H-HP-0.113500        0    -6.06961  -2.52222  -16.11396  L
H-H-0.340000         0    -4.09901  -2.25853  -14.72097  L
H-H-0.340000         0    -4.05167  -0.66809  -14.99133  L
H-H-0.340000         0    -3.75661  -1.71275  -16.25192  L
N-N--0.415700        0    -9.82193   1.27204  -10.88446  L
C-CT--0.003100       -1   -10.32273   1.68048  -9.57342  L
C-C-0.597300         0    -11.26682   2.8875   -9.82606  L
N-N--0.415700        0    -10.78357   3.93369  -10.52259  L
C-CT--0.149000       -1   -11.5434   5.02453  -11.1538  L
O-O--0.567900        0    -12.44227   2.81723  -9.4832   L
C-CT--0.003600       0    -9.19874   2.01065  -8.59271  L
C-CT--0.064500       0    -8.72756   0.71549  -7.93394  L
C-C-0.695100         0    -7.54977   0.9411   -7.01326  L
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O-O--0.608600        0    -7.37287   1.98092  -6.39815  L
N-N--0.940700        0    -6.68755  -0.03524  -6.88558  L
H-H-0.271900         0    -9.63922   2.02983  -11.52483  L
H-H-0.271900         0    -9.78343   3.93652  -10.68304  L
H-H1-0.085000        0    -10.94353   0.88509  -9.15436  L
H-HC-0.017100        0    -9.57909   2.68004  -7.81961  L
H-HC-0.017100        0    -8.37142   2.49989  -9.10433  L
H-HC-0.035200        0    -8.43545   0.0075   -8.70642  L
H-HC-0.035200        0    -9.54347   0.28862  -7.3518   L
H-H-0.425100         0    -5.99071   0.07415  -6.15385  L
H-H-0.425100         0    -6.86357  -0.92112  -7.32     L
H-H1-0.097600        0    -11.6361   5.8558   -10.45197  L
H-H1-0.097600        0    -12.544    4.67806  -11.42083  L
H-H1-0.097600        0    -11.02896   5.37077  -12.05091  L
N-N--0.415700        0    -5.36115   11.33258  -6.84186  L
C-CT--0.002400       -1   -4.40335   10.31966  -6.40183  L
C-C-0.597300         0    -2.95352   10.84195  -6.37056  L
O-O--0.567900        0    -2.68466   11.95604  -6.81148  L
C-CT--0.034300       0    -4.46888   9.10477  -7.34697  L
C-CA-0.011800        0    -5.72124   8.25465  -7.30624  L
C-CA--0.125600       0    -5.74753   7.08097  -6.5266   L
C-CA--0.170400       0    -6.8301    8.58339  -8.10735  L
C-CA--0.107200       0    -6.88157   6.24978  -6.54192  L
C-CA--0.170400       0    -7.96077   7.75181  -8.11927  L
C-CA--0.125600       0    -7.98544   6.58202  -7.34064  L
H-H-0.271900         0    -6.29063   11.04092  -7.11858  L
H-H-0.271900         0    -4.97338   12.20834  -7.17701  L
H-H1-0.097800        0    -4.66887   10.00271  -5.39728  L
H-HC-0.029500        0    -3.64258   8.44017  -7.10351  L
H-HC-0.029500        0    -4.31231   9.44823  -8.37069  L
H-HA-0.133000        0    -4.90428   6.81898  -5.9051   L
H-HA-0.143000        0    -6.82649   9.45794  -8.73941  L
H-HA-0.129700        0    -6.92873   5.36242  -5.92962  L
H-HA--0.170400       0    -8.7989    8.01506  -8.74551  L
H-HA--0.125600       0    -8.84627   5.93024  -7.34955  L
N-N--0.415700        0    -2.02263   10.01365  -5.88449  L
C-CT--0.023700       -1   -0.57285   10.10909  -6.11793  L
C-C-0.597300         0     0.05709   8.72942  -5.93611  L
O-O--0.567900        0    -0.41697   7.93827  -5.1175   L
C-CT-0.034200        0     0.0435    11.10598  -5.11866  L
C-CT-0.001800        0     1.48491   11.50395  -5.45024  L
S-S--0.273700        0     2.20334   12.63271  -4.22771  L
C-CT--0.053600       0     3.69043   13.16348  -5.11644  L
H-H-0.271900         0    -2.34511   9.13059  -5.50579  L
H-H1-0.088000        0    -0.39896   10.45752  -7.13772  L
H-HC-0.024100        0     0.02038   10.67257  -4.11841  L
H-HC-0.024100        0    -0.55099   12.01942  -5.11371  L
H-H1-0.044000        0     1.49345   11.99187  -6.42557  L
H-H1-0.044000        0     2.11233   10.6146  -5.49792  L
H-H1-0.068400        0     4.26417   13.84359  -4.48646  L
H-H1-0.068400        0     3.40384   13.68048  -6.03262  L
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H-H1-0.068400        0     4.30365   12.29867  -5.36527  L
N-N--0.415700        0     1.11486   8.44715  -6.69402  L
C-CT--0.058100       -1    1.67559   7.10632  -6.85391  L
C-C-0.597300         0     3.21052   7.16951  -6.77385  L
O-O--0.567900        0     3.90728   7.14905  -7.78524  L
C-CT--0.007400       0     1.18692   6.51618  -8.18865  L
C-CC-0.186800        0    -0.24845   6.82673  -8.51218  L
N-NB--0.543200       0    -0.67489   7.94616  -9.22349  L
C-CW--0.220700       0    -1.32623   6.06724  -8.17883  L
C-CR-0.163500        0    -1.99915   7.82184  -9.34896  L
N-NA--0.279500       0    -2.4172    6.70595  -8.7282   L
H-H-0.271900         0     1.39135   9.13599  -7.37786  L
H-H1-0.136000        0     1.31965   6.45353  -6.05848  L
H-HC-0.036700        0     1.31891   5.43606  -8.16547  L
H-HC-0.036700        0     1.78227   6.91365  -9.01135  L
H-H4-0.186200        0    -1.29097   5.13298  -7.64016  L
H-H-0.333900         0    -3.36964   6.3511   -8.77167  L
H-H5-0.143500        0    -2.6303    8.51189  -9.8945   L
N-N--0.415700        0     3.75147   7.3271   -5.56582  L
C-CT--0.059700       -1    5.16426   7.67172  -5.35679  L
C-C-0.597300         0     6.11762   6.5083   -5.69548  L
O-O--0.567900        0     5.82364   5.35912  -5.35271  L
C-CT-0.130300        0     5.41147   8.21971  -3.9273   L
C-CT--0.043000       0     5.13218   7.2057   -2.79309  L
C-CT--0.320400       0     4.58971   9.50667  -3.73295  L
C-CT--0.066000       0     5.48015   7.71589  -1.38876  L
H-H-0.271900         0     3.12687   7.28258  -4.76708  L
H-H1-0.086900        0     5.35985   8.4923   -6.03922  L
H-HC-0.018700        0     6.46569   8.49657  -3.8692   L
H-HC-0.023600        0     5.71161   6.3043   -2.97072  L
H-HC-0.023600        0     4.08423   6.92732  -2.79426  L
H-HC-0.088200        0     3.52696   9.27634  -3.64636  L
H-HC-0.088200        0     4.74445   10.18022  -4.57424  L
H-HC-0.088200        0     4.90954   10.02175  -2.82778  L
H-HC-0.018600        0     4.77162   8.48553  -1.08375  L
H-HC-0.018600        0     6.48936   8.12688  -1.37618  L
H-HC-0.018600        0     5.41782   6.89054  -0.6792   L
N-N--0.254800        0     7.25984   6.76898  -6.35935  L
C-CT--0.026600       -1    8.09643   5.71968  -6.93533  L
C-C-0.589600         0     8.57607   4.58841  -6.03574  L
O-O--0.574800        0     8.75416   4.78275  -4.8321   L
C-CT--0.007000       0     9.29125   6.44175  -7.55867  L
C-CT-0.018900        0     8.7143    7.78928  -7.96213  L
C-CT-0.019200        0     7.70931   8.07184  -6.84957  L
H-H1-0.064100        0     7.531     5.28201  -7.74852  L
H-HC-0.025300        0     9.6675    5.90139  -8.42687  L
H-HC-0.025300        0     10.07573   6.58918  -6.8144   L
H-HC-0.021300        0     8.18853   7.69021  -8.91354  L
H-HC-0.021300        0     9.48238   8.56062  -8.02446  L
H-H1-0.039100        0     8.1937    8.61858  -6.03968  L
H-H1-0.039100        0     6.89756   8.66104  -7.27409  L
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N-N--0.415700        0     8.83492   3.42432  -6.63564  L
C-CT--0.051800       -1    9.25216   2.20168  -5.94497  L
C-C-0.597300         0     10.48761   2.39585  -5.03935  L
O-O--0.567900        0     11.52122   2.9028   -5.47738  L
C-CT--0.110200       0     9.47734   1.06449  -6.94972  L
C-CT-0.353100        0     8.23842   0.62038  -7.74897  L
C-CT--0.412100       0     8.60195  -0.57334  -8.63186  L
C-CT--0.412100       0     7.06688   0.22515  -6.85197  L
H-H-0.271900         0     8.66912   3.38875  -7.64314  L
H-H1-0.092200        0     8.4343    1.90884  -5.29224  L
H-HC-0.045700        0     9.84667   0.20345  -6.39287  L
H-HC-0.045700        0     10.25121   1.37839  -7.65038  L
H-HC--0.036100       0     7.90284   1.42127  -8.39489  L
H-HC-0.100000        0     8.98631  -1.38847  -8.02427  L
H-HC-0.100000        0     9.36021  -0.26136  -9.35146  L
H-HC-0.100000        0     7.7247   -0.9042   -9.18709  L
H-HC-0.100000        0     7.38671  -0.47876  -6.08646  L
H-HC-0.100000        0     6.29136  -0.22095  -7.47072  L
H-HC-0.100000        0     6.65055   1.11183  -6.37599  L
N-N--0.415700        0     10.38952   1.9321   -3.78546  L
C-CT--0.059700       -1    11.54125   1.5052   -2.969    L
C-C-0.597300         0     11.89143   0.09104  -3.44346  L
O-O--0.567900        0     11.04692  -0.81214  -3.41478  L
C-CT-0.130300        0     11.21204   1.55108  -1.46072  L
C-CT--0.043000       0     10.74119   2.94628  -0.98274  L
C-CT--0.320400       0     12.42038   1.08655  -0.62786  L
C-CT--0.066000       0     11.64271   4.12728  -1.36788  L
H-H-0.271900         0     9.48031   1.56435  -3.5257   L
H-H1-0.086900        0     12.38792   2.16351  -3.16721  L
H-HC-0.018700        0     10.39587   0.85261  -1.26752  L
H-HC-0.023600        0     10.6539   2.93791   0.1031   L
H-HC-0.023600        0     9.74517   3.13215  -1.38363  L
H-HC-0.088200        0     12.64587   0.0421   -0.84487  L
H-HC-0.088200        0     12.19612   1.17032   0.43562  L
H-HC-0.088200        0     13.29796   1.69131  -0.85916  L
H-HC-0.018600        0     11.27756   5.03209  -0.88342  L
H-HC-0.018600        0     11.61796   4.28034  -2.44644  L
H-HC-0.018600        0     12.66755   3.95005  -1.04335  L
N-N--0.415700        0     13.11254  -0.08022  -3.9405   L
C-CT--0.051800       -1    13.54363  -1.21932  -4.74413  L
C-C-0.597300         0     14.59367  -2.07296  -4.04903  L
O-O--0.567900        0     15.36646  -1.60403  -3.2167   L
C-CT--0.110200       0     14.11214  -0.72388  -6.09638  L
C-CT-0.353100        0     13.15219   0.03599  -7.0273   L
C-CT--0.412100       0     13.94627   0.74336  -8.12634  L
C-CT--0.412100       0     12.17724  -0.9163   -7.71286  L
H-H-0.271900         0     13.7126   0.73843  -3.94794  L
H-H1-0.092200        0     12.68002  -1.85046  -4.94255  L
H-HC-0.045700        0     14.51157  -1.57681  -6.64657  L
H-HC-0.045700        0     14.95156  -0.06927  -5.88716  L
H-HC--0.036100       0     12.59763   0.78126  -6.4649   L
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H-HC-0.100000        0     14.49544   0.01887  -8.72705  L
H-HC-0.100000        0     14.64911   1.44665  -7.68286  L
H-HC-0.100000        0     13.26324   1.29901  -8.77122  L
H-HC-0.100000        0     11.56627  -0.36012  -8.4226   L
H-HC-0.100000        0     11.53205  -1.37387  -6.96776  L
H-HC-0.100000        0     12.72551  -1.67817  -8.25946  L
N-N--0.415700        0     14.66971  -3.32158  -4.48232  L
C-CT--0.025200       -1    15.78311  -4.20641  -4.22048  L
C-C-0.597300         0     15.80172  -5.43402  -5.13986  L
N-N--0.415700        0     16.57464  -6.45404  -4.75541  L
C-CT--0.149000       0     16.80669  -7.67279  -5.52832  L
O-O--0.567900        0     15.13469  -5.46646  -6.18131  L
H-H-0.271900         0     13.97287  -3.62637  -5.15422  L
H-H-0.271900         0     17.04085  -6.36467  -3.85363  L
H-H1-0.069800        0     15.74381  -4.54755  -3.18759  L
H-H1-0.069800        0     16.71749  -3.66254  -4.36268  L
H-H1-0.097600        0     17.45277  -7.44991  -6.37996  L
H-H1-0.097600        0     15.86215  -8.07428  -5.89687  L
H-H1-0.097600        0     17.29657  -8.42039  -4.90131  L
N-N--0.415700        0     13.7667  -4.17022  -8.55982  L
C-CT--0.038900       -1    12.37816  -4.64748  -8.42194  L
C-C-0.597300         0     11.74965  -4.20045  -7.08661  L
O-O--0.567900        0     12.51272  -3.90635  -6.16919  L
C-CT-0.365400        0     12.33249  -6.18705  -8.51773  L
O-OH--0.676100       0     13.09657  -6.83083  -7.51632  L
C-CT--0.243800       0     12.83561  -6.7039   -9.86436  L
H-H-0.271900         0     14.36486  -4.19392  -7.73708  L
H-H-0.271900         0     14.12663  -3.85132  -9.45018  L
H-H1-0.100700        0     11.78003  -4.23064  -9.23174  L
H-H1-0.004300        0     11.30451  -6.51544  -8.40554  L
H-HC-0.064200        0     12.6902  -7.78295  -9.91632  L
H-HC-0.064200        0     13.89656  -6.48531  -9.98819  L
H-HC-0.064200        0     12.27215  -6.23731  -10.67264  L
H-HO-0.410200        0     13.80912  -6.22681  -7.23498  L
N-N--0.254800        0     10.41103  -4.11786  -6.92061  L
C-CT--0.026600       -1    9.79257  -3.62487  -5.67867  L
C-C-0.589600         0     10.18794  -4.47187  -4.46941  L
O-O--0.574800        0     10.05237  -5.69659  -4.47259  L
C-CT--0.007000       0     8.28166  -3.62679  -5.92399  L
C-CT-0.018900        0     8.10115  -4.64077  -7.04969  L
C-CT-0.019200        0     9.37156  -4.46304  -7.8808   L
H-H1-0.064100        0     10.11029  -2.59681  -5.50079  L
H-HC-0.025300        0     7.96701  -2.64622  -6.27355  L
H-HC-0.025300        0     7.72188  -3.90129  -5.03004  L
H-HC-0.021300        0     7.20074  -4.44615  -7.63321  L
H-HC-0.021300        0     8.07891  -5.64636  -6.62806  L
H-H1-0.039100        0     9.58691  -5.38183  -8.42046  L
H-H1-0.039100        0     9.23928  -3.64205  -8.58619  L
N-N--0.415700        0     10.71359  -3.8077   -3.4426   L
C-CT--0.051800       -1    11.18047  -4.43941  -2.21476  L
C-C-0.597300         0     10.02243  -5.03211  -1.41108  L
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 O-O--0.567900        0     8.97753  -4.39459  -1.27299  L
 C-CT--0.110200       0     11.91431  -3.36473  -1.38989  L
 C-CT-0.353100        0     12.85328  -3.94355  -0.31718  L
 C-CT--0.412100       0     14.1802  -4.37374  -0.94206  L
 C-CT--0.412100       0     13.14065  -2.87904   0.73649  L
 H-H-0.271900         0     10.78717  -2.79937  -3.51195  L
 H-H1-0.092200        0     11.87774  -5.23315  -2.48042  L
 H-HC-0.045700        0     11.16389  -2.73016  -0.91426  L
 H-HC-0.045700        0     12.50288  -2.72852  -2.05192  L
 H-HC--0.036100       0     12.38838  -4.79703   0.17523  L
 H-HC-0.100000        0     14.64746  -3.52252  -1.43564  L
 H-HC-0.100000        0     14.01204  -5.17168  -1.66395  L
 H-HC-0.100000        0     14.86545  -4.73478  -0.17908  L
 H-HC-0.100000        0     13.5805  -1.99876   0.26948  L
 H-HC-0.100000        0     13.83047  -3.26715   1.48438  L
 H-HC-0.100000        0     12.20609  -2.6061    1.22485  L
 N-N--0.415700        0     10.22742  -6.23243  -0.86788  L
 C-CT--0.024900       -1    9.27643  -6.904     0.01351  L
 C-C-0.597300         0     9.96905  -7.89284   0.96055  L
 O-O--0.567900        0     11.18517  -7.87557   1.16543  L
 C-CT-0.211700        0     8.16517  -7.52274  -0.85458  L
 O-OH--0.654600       0     7.06721  -7.94536  -0.05988  L
 H-H-0.271900         0     11.10616  -6.70733  -1.04983  L
 H-H1-0.084300        0     8.81052  -6.14262   0.64136  L
 H-H1-0.035200        0     8.57004  -8.3671   -1.41417  L
 H-H1-0.035200        0     7.8059   -6.77827  -1.56671  L
 H-HO-0.427500        0     6.30163  -7.34927  -0.235    L
 N-N--0.347900        0     9.15774  -8.73465   1.58913  L
 C-CT--0.240000       -1    9.47045  -9.78641   2.55491  L
 C-C-0.734100         0     10.40477  -10.85652   1.97724  L
 O-O--0.589400        0     11.36246  -11.24214   2.64066  L
 C-CT--0.009400       0     8.10723  -10.3452   3.04563  L
 C-CT-0.018700        0     7.21877  -9.2907    3.76649  L    H-HC
1455  0.        0.
 C-CT--0.047900       0     5.69199  -9.45134   3.59774  H
 C-CT--0.014300       0     5.15848  -8.95831   2.25494  H
 N-N3--0.385400       0     3.6449   -8.97171   2.23199  H
 H-H-0.274700         0     8.18934  -8.62945   1.30675  L
 H-H1-0.142600        0     9.99809  -9.34764   3.40388  L
 H-HC-0.036200        0     8.28686  -11.17448   3.73194  L
 H-HC-0.036200        0     7.56155  -10.7457   2.19196  L
 H-HC-0.010300        0     7.47659  -8.28091   3.44693  L
 H-HC-0.010300        0     7.44987  -9.34384   4.83141  L
 H-HC-0.062100        0     5.22555  -8.86221   4.39426  H
 H-HC-0.062100        0     5.42929  -10.50107   3.75526  H
 H-HP-0.113500        0     5.48996  -9.58446   1.42637  H
 H-HP-0.113500        0     5.44901  -7.92941   2.0462   H
 H-H-0.340000         0     3.24995  -9.54601   2.99219  H
 H-H-0.340000         0     3.27952  -9.39065   1.36678  H
 H-H-0.340000         0     3.10556  -7.99645   2.29814  H
 N-N--0.347900        0     10.18459  -11.22147   0.70715  L
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C-CT--0.263700       -1    11.11166  -11.81755  -0.28337  L
C-C-0.734100         0     12.60355  -11.5383  -0.04954  L
O-O--0.589400        0     13.42761  -12.4026  -0.32153  L
C-CT--0.000700       0     10.6358  -11.30761  -1.65588  L
C-CT-0.039000        0     11.57763  -11.54752  -2.84576  L
C-CT-0.048600        0     10.9019  -10.98214  -4.10016  L
N-N2--0.529500       0     11.85512  -10.74672  -5.20058  L
C-CA-0.807600        0     11.76257  -9.79145  -6.11132  L
N-N2--0.862700       0     10.77975  -8.94318  -6.14752  L
N-N2--0.862700       0     12.68712  -9.64374  -7.01287  L
H-H-0.274700         0     9.28763  -10.90769   0.34472  L
H-H1-0.156000        0     11.00928  -12.90365  -0.2593   L
H-HC-0.032700        0     10.47442  -10.22978  -1.57851  L
H-HC-0.032700        0     9.67186  -11.77081  -1.87541  L
H-HC-0.028500        0     11.77256  -12.61343  -2.97076  L
H-HC-0.028500        0     12.51722  -11.01897  -2.67892  L
H-H1-0.068700        0     10.43966  -10.03694  -3.82343  L
H-H1-0.068700        0     10.11329  -11.66364  -4.42608  L
H-H-0.345600         0     12.65066  -11.358   -5.25395  L
H-H-0.447800         0     10.57214  -8.40402  -6.9812   L
H-H-0.447800         0     10.07142  -8.94026  -5.41529  L
H-H-0.447800         0     12.68679  -8.75712  -7.50658  L
H-H-0.447800         0     13.45998  -10.27511  -7.08742  L
N-N--0.415700        0     12.95568  -10.32801   0.37975  L
C-CT--0.058100       -1    14.3286  -9.8231    0.46376  L
C-C-0.597300         0     14.94082  -9.8185    1.8729   L
N-N--0.415700        0     14.22656  -10.32817   2.88448  L
C-CT--0.149000       0     14.68501  -10.44758   4.2663   L
O-O--0.567900        0     16.06854  -9.3439    2.02837  L
C-CT--0.007400       0     14.29792  -8.3963   -0.11854  L
C-CC-0.186800        0     13.75756  -8.24034  -1.52359  L
N-NB--0.543200       0     12.41289  -8.07248  -1.85815  L
C-CW--0.220700       0     14.50924  -8.07136  -2.64877  L
C-CR-0.163500        0     12.38144  -7.81605  -3.17373  L
N-NA--0.279500       0     13.62733  -7.80176  -3.67685  L
H-H-0.271900         0     12.20907  -9.66203   0.52667  L
H-H-0.271900         0     13.30814  -10.69836   2.65831  L
H-H1-0.136000        0     14.98418  -10.43386  -0.15938  L
H-HC-0.036700        0     15.29643  -7.96689  -0.09303  L
H-HC-0.036700        0     13.66656  -7.79526   0.52736  L
H-H4-0.186200        0     15.59035  -8.08404  -2.68652  L
H-H-0.333900         0     13.85879  -7.56037  -4.63219  L
H-H5-0.143500        0     11.48123  -7.61396  -3.73972  L
H-H1-0.097600        0     15.40882  -9.66413   4.49598  L
H-H1-0.097600        0     15.16262  -11.41885   4.40822  L
H-H1-0.097600        0     13.83389  -10.36767   4.94405  L
N-N--0.415700        0     14.60566  -6.79283   5.46824  L
C-CT--0.038900       -1    13.92216  -5.61224   4.90815  L
C-C-0.597300         0     12.72799  -5.10822   5.7334   L
O-O--0.567900        0     12.15266  -4.06038   5.42289  L
C-CT-0.365400        0     13.44409  -5.8902    3.47458  L
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O-OH--0.676100       0     12.74929  -7.11972   3.42715  L
C-CT--0.243800       0     14.64128  -5.96283   2.53438  L
H-H-0.271900         0     14.40072  -7.68044   5.02031  L
H-H-0.271900         0     15.39568  -6.69352   6.09311  L
H-H1-0.100700        0     14.62887  -4.7837    4.87213  L
H-H1-0.004300        0     12.78839  -5.08576   3.139    L
H-HC-0.064200        0     14.28117  -6.01487   1.51482  L
H-HC-0.064200        0     15.24901  -6.84083   2.75332  L
H-HC-0.064200        0     15.2524   -5.06593   2.63552  L
H-HO-0.410200        0     12.36198  -7.23997   2.54413  L
N-N--0.415700        0     12.36883  -5.81847   6.8057   L
C-CT--0.024900       -1    11.46931  -5.34035   7.86205  L
C-C-0.597300         0     11.99491  -4.0599    8.508    L
O-O--0.567900        0     13.2002   -3.93233   8.70925  L
C-CT-0.211700        0     11.31382  -6.41952   8.93612  L
O-OH--0.654600       0     12.58538  -6.85379   9.38123  L
H-H-0.271900         0     12.9047   -6.64926   7.01097  L
H-H1-0.084300        0     10.4963   -5.14784   7.42216  L
H-H1-0.035200        0     10.77499  -7.27008   8.51637  L
H-H1-0.035200        0     10.74261  -6.02252   9.77702  L
H-HO-0.427500        0     13.10697  -6.07731   9.63281  L
N-N--0.415700        0     11.09421  -3.14717   8.87769  L
C-CT--0.087500       -1    11.43516  -1.92002   9.62644  L
C-C-0.597300         0     12.15199  -2.22804   10.94971  L
N-N--0.415700        0     11.67261  -3.23605   11.69677  L
O-O--0.567900        0     13.10341  -1.53461   11.29879  L
C-CT-0.298500        0     10.1818   -1.07315   9.89988  L
C-CT--0.319200       0     10.46706   0.20254   10.70586  L
C-CT--0.319200       0     9.54607   -0.62612   8.58474  L
H-H-0.271900         0     10.12069  -3.3571    8.68695  L
H-H-0.096900         0     10.87952  -3.75268   11.3489  L
H-H1-0.096900        0     12.12902  -1.32913   9.02827  L
H-HC--0.029700       0     9.4541    -1.67396   10.44759  L
H-HC-0.079100        0     9.56047    0.79876   10.80419  L
H-HC-0.079100        0     11.23914   0.79304   10.21108  L
H-HC-0.079100        0     10.81139  -0.05447   11.70818  L
H-HC-0.079100        0     9.26627   -1.48582   7.97906  L
H-HC-0.079100        0     10.23862   0.00224   8.02517  L
H-HC-0.079100        0     8.65141   -0.06298   8.82577  L
N-N--0.415700        0     14.05482   7.17322   5.63951  L
C-CT--0.051800       -1    13.43988   6.51318   4.47996  L
C-C-0.597300         0     12.88683   7.48984   3.4234   L
O-O--0.567900        0     12.63403   7.07335   2.29916  L
C-CT--0.110200       0     12.32657   5.5549    4.94973  L
C-CT-0.353100        0     12.75213   4.44958   5.93588  L
C-CT--0.412100       0     11.53355   3.60288   6.3041   L
C-CT--0.412100       0     13.82305   3.53238   5.34332  L
H-H-0.271900         0     13.55485   7.1935    6.52041  L
H-H-0.271900         0     15.05244   7.35191   5.63673  L
H-H1-0.092200        0     14.20442   5.92323   3.97302  L
H-HC-0.045700        0     11.90972   5.07234   4.0656   L
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H-HC-0.045700        0     11.53191   6.14334   5.40969  L
H-HC--0.036100       0     13.14003   4.90333   6.84786  L
H-HC-0.100000        0     11.82098   2.83556   7.02317  L
H-HC-0.100000        0     11.12566   3.12775   5.41297  L
H-HC-0.100000        0     10.7669    4.2326    6.75536  L
H-HC-0.100000        0     14.01114   2.69933   6.02172  L
H-HC-0.100000        0     14.75564   4.07997   5.21579  L
H-HC-0.100000        0     13.4948    3.1456    4.37891  L
N-N--0.415700        0     12.71434   8.77209   3.75936  L
C-CT-0.033700        0     12.35582   9.83096   2.80798  L
C-C-0.597300         0     13.50817   10.15725   1.83117  L
N-N--0.415700        0     14.72071   10.38125   2.35802  L
C-CT--0.149000       -1    15.9423    10.65621   1.60006  L
O-O--0.567900        0     13.30309   10.19998   0.61923  L
C-CT--0.182500       0     11.91005   11.06776   3.59899  L
H-H-0.271900         0     12.89348   9.02887   4.71629  L
H-H-0.271900         0     14.78038   10.37564   3.36329  L
H-H1-0.082300        0     11.51052   9.49114   2.20531  L
H-HC-0.060300        0     12.72197   11.4381   4.2261   L
H-HC-0.060300        0     11.0527    10.81905   4.22628  L
H-HC-0.060300        0     11.613     11.85534   2.90399  L
H-H1-0.097600        0     15.69981   11.03184   0.60327  L
H-H1-0.097600        0     16.53421   9.7451    1.50916  L
H-H1-0.097600        0     16.53626   11.41372   2.11537  L
N-N--0.415700        0     14.83901   7.19932   0.54037  L
C-CT--0.051800       -1    15.10974   7.88774  -0.71808  L
C-C-0.597300         0     13.83969   8.05847  -1.56721  L
O-O--0.567900        0     12.80251   7.45637  -1.28949  L
C-CT--0.110200       0     16.18023   7.08839  -1.4964   L
C-CT-0.353100        0     17.57885   7.04708  -0.85331  L
C-CT--0.412100       0     18.4471    6.02298  -1.58291  L
C-CT--0.412100       0     18.28104   8.4037   -0.93191  L
H-H-0.271900         0     13.86977   7.1877    0.85925  L
H-H-0.271900         0     15.46933   6.47756   0.85585  L
H-H1-0.092200        0     15.48465   8.88694  -0.50345  L
H-HC-0.045700        0     16.28765   7.50531  -2.49803  L
H-HC-0.045700        0     15.81967   6.06423  -1.60825  L
H-HC--0.036100       0     17.49567   6.7461    0.19121  L
H-HC-0.100000        0     19.4341    5.97772  -1.12178  L
H-HC-0.100000        0     18.55884   6.2979   -2.63219  L
H-HC-0.100000        0     17.99268   5.0333   -1.52235  L
H-HC-0.100000        0     18.39361   8.71088  -1.97233  L
H-HC-0.100000        0     19.27138   8.32889  -0.481    L
H-HC-0.100000        0     17.71647   9.16053  -0.39361  L
N-N--0.415700        0     13.94303   8.84454  -2.63958  L
C-CT--0.025200       -1    12.93444   8.9804   -3.69357  L
C-C-0.597300         0     12.91634   10.39192  -4.28828  L
N-N--0.415700        0     12.65873   10.50544  -5.59588  L
C-CT--0.149000       0     12.60292   11.77967  -6.31163  L
O-O--0.567900        0     13.12084   11.36283  -3.56105  L
H-H-0.271900         0     14.7949    9.37433  -2.7481   L
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H-H-0.271900          0     12.51397   9.66099  -6.12724  L
H-H1-0.069800         0     11.94289   8.7749   -3.29444  L
H-H1-0.069800         0     13.1431   8.26011  -4.48383  L
H-H1-0.097600         0     11.8267   12.41562  -5.8807   L
H-H1-0.097600         0     12.38331   11.61354  -7.36776  L
H-H1-0.097600         0     13.56112   12.29684  -6.22516  L
N-N--0.415700         0     12.21317   5.47898  -9.55997  L
C-CT--0.025200        -1    12.3321   4.65307  -8.3616   L
C-C-0.597300          0     13.75909   4.628    -7.80635  L
O-O--0.567900         0     14.67103   5.19587  -8.40533  L
H-H-0.271900          0     11.414    5.34407  -10.17898  L
H-H-0.271900          0     13.06827   5.87829  -9.92835  L
H-H1-0.069800         0     12.04078   3.63008  -8.59821  L
H-H1-0.069800         0     11.66864   5.02663  -7.58524  L
N-N--0.415700         0     13.95652   4.01203  -6.63724  L
C-CT--0.087500        -1    15.2179   4.07168  -5.87229  L
C-C-0.597300          0     15.50578   2.78434  -5.103    L
O-O--0.567900         0     14.61923   2.2013   -4.48641  L
C-CT-0.298500         0     15.21187   5.24749  -4.87047  L
C-CT--0.319200        0     15.34052   6.6048   -5.57123  L
C-CT--0.319200        0     13.95983   5.27857  -3.98275  L
H-H-0.271900          0     13.1582   3.55276  -6.20253  L
H-H1-0.096900         0     16.04314   4.2267   -6.56811  L
H-HC--0.029700        0     16.08258   5.14255  -4.22162  L
H-HC-0.079100         0     16.20512   6.59412  -6.23615  L
H-HC-0.079100         0     15.47972   7.39291  -4.83349  L
H-HC-0.079100         0     14.44884   6.81613  -6.16039  L
H-HC-0.079100         0     14.02991   6.10047  -3.28337  L
H-HC-0.079100         0     13.88197   4.35724  -3.40919  L
H-HC-0.079100         0     13.05779   5.40269  -4.58178  L
N-N--0.415700         0     16.76075   2.3368   -5.11463  L
C-CT--0.059700        -1    17.20416   1.12503  -4.41033  L
C-C-0.597300          0     17.40768   1.39251  -2.92094  L
O-O--0.567900         0     17.9834   2.40363  -2.51728  L
C-CT-0.130300         0     18.47424   0.54519  -5.08401  L
C-CT--0.043000        0     18.15163   0.12992  -6.54277  L
C-CT--0.320400        0     19.01882  -0.66937  -4.30469  L
C-CT--0.066000        0     19.37824  -0.25543  -7.38016  L
H-H-0.271900          0     17.45483   2.88198  -5.60216  L
H-H1-0.086900         0     16.42683   0.37038  -4.487    L
H-HC-0.018700         0     19.2444   1.31895  -5.09829  L
H-HC-0.023600         0     17.67165   0.95901  -7.06226  L
H-HC-0.023600         0     17.45109  -0.70654  -6.53635  L
H-HC-0.088200         0     19.89664  -1.08173  -4.79995  L
H-HC-0.088200         0     18.25548  -1.44432  -4.22405  L
H-HC-0.088200         0     19.33928  -0.37353  -3.3057   L
H-HC-0.018600         0     20.12475   0.53827  -7.33488  L
H-HC-0.018600         0     19.07419  -0.39494  -8.41798  L
H-HC-0.018600         0     19.81264  -1.18837  -7.02289  L
N-N--0.415700         0     16.94661   0.45376  -2.09906  L
C-CT--0.002400        -1    17.23088   0.41281  -0.67777  L
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C-C-0.597300          0     18.69331  -0.00392  -0.39821  L
N-N--0.415700         0     19.60159   0.98256  -0.34987  L
C-CT--0.149000       -1     21.0274    0.82157  -0.04124  L
O-O--0.567900         0     18.99368  -1.18553  -0.23866  L
C-CT--0.034300        0     16.20137  -0.48287   0.02658  L
C-CA-0.011800         0     16.30455  -0.43801   1.53965  L
C-CA--0.125600        0     15.94058   0.7314    2.23613  L
C-CA--0.125600        0     16.80112  -1.54648   2.25069  L
C-CA--0.170400        0     16.07878   0.79305   3.63505  L
C-CA--0.170400        0     16.92865  -1.48863   3.65008  L
C-CA--0.107200        0     16.56978  -0.3188    4.34216  L
H-H-0.271900          0     16.47032  -0.34542  -2.50456  L
H-H-0.271900          0     19.26657   1.89678  -0.62283  L
H-H1-0.097800         0     17.10478   1.42018  -0.28093  L
H-HC-0.029500         0     16.31648  -1.51084  -0.32182  L
H-HC-0.029500         0     15.20096  -0.15264  -0.25425  L
H-HA-0.133000         0     15.56439   1.58703   1.69512  L
H-HA-0.133000         0     17.11116  -2.43506   1.71798  L
H-HA-0.143000         0     15.8135    1.69294   4.16972  L
H-HA-0.143000         0     17.32581  -2.33607   4.19132  L
H-HA-0.129700         0     16.68376  -0.27346   5.41682  L
H-H1-0.097600         0     21.47754   0.11439  -0.7409   L
H-H1-0.097600         0     21.14392   0.43014   0.97119  L
H-H1-0.097600         0     21.54241   1.78004  -0.11976  L
C-CT-0.055800         0    -6.65368  -9.76454  -6.42648  L
C-CT-0.106500         0    -6.10163  -10.89069  -5.55173  L
O-OS--0.354800        0    -4.89745  -11.37294  -6.13497  L
C-CT-0.202200         0    -5.74368  -10.52217  -4.10377  L
O-OS--0.495400        0    -6.81622  -10.52687  -3.17091  L
C-CT-0.067000         0    -4.81292  -11.70341  -3.79729  L
O-OH--0.613900        0    -5.53563  -12.91855  -3.59307  L
C-CT-0.006600         0    -4.03318  -11.85694  -5.10668  L
N-N*--0.048400        0    -2.72768  -11.12338  -5.10364  L
C-C-0.753800          0    -1.58628  -11.78118  -4.63324  L
O-O--0.625800         0    -1.63065  -12.91754  -4.16104  L
N-NC--0.758400        0    -0.36829  -11.13099  -4.70379  L
C-CA--0.521500        0    -0.25081  -9.93568  -5.22797  L
N-N2--0.953800        0     0.96329  -9.50007  -5.43044  L
C-CM--0.521500        0    -1.38249  -9.25166  -5.72964  L
C-CM-0.005300         0    -2.59343  -9.86414  -5.64413  L
H-HC-0.067900         0    -7.56941  -9.36294  -6.00398  L
H-HC-0.067900         0    -5.91333  -8.97522  -6.51937  L
H-H1-0.117400         0    -6.82256  -11.70814  -5.52434  L
H-H1-0.061500         0    -5.16798  -9.59634  -4.06653  L
H-H1-0.097200         0    -4.15324  -11.49276  -2.95579  L
H-HO-0.418600         0    -5.7216   -13.04502  -2.63356  L
H-H2-0.202900         0    -3.82796  -12.92217  -5.25445  L
H-H-0.423900          0     1.77502  -10.08345  -5.22807  L
H-H-0.423900          0     1.18468  -8.64717  -5.95654  L
H-HA-0.192800         0    -1.37587  -8.27791  -6.20293  L
H-H4-0.195800         0    -3.46173  -9.36236  -6.04468  L
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 P-P-1.166200          0    -7.55733  -9.20896  -2.67471  L
 O-O2--0.776000        0    -8.29703  -9.61877  -1.46497  L
 O-O2--0.776000        0    -8.34403  -8.67271  -3.79959  L
 O-OS--0.498900        0    -6.41745  -8.14489  -2.2935   L
 C-CT-0.055800         0    -5.52563  -8.27238  -1.18666  L    H-H1
1732  0.        0.
 C-CT-0.106500         0    -4.36389  -7.24631  -1.25586  H
 O-OS--0.354800        0    -3.5609   -7.59865  -2.38294  H
 C-CT-0.202200         0    -4.77273  -5.79749  -1.53284  H
 O-OH--0.654100        0    -5.18619  -5.03372  -0.44302  H
 C-CT-0.067000         0    -3.58137  -5.19994  -2.29289  H
 O-OH--0.613900        0    -2.50247  -4.67783  -1.52893  H
 C-CT-0.039400         0    -3.05625  -6.45763  -3.03405  H
 N-N*--0.025100        0    -3.51436  -6.49596  -4.41175  H
 C-CK-0.200600         0    -4.78538  -6.83107  -4.82383  H
 N-NB--0.607300        0    -5.02303  -6.58375  -6.08199  H
 C-CB-0.051500         0    -3.84333  -6.03656  -6.5313   H
 C-CA-0.700900         0    -3.48612  -5.44753  -7.75735  H
 N-N2--0.901900        0    -4.38835  -5.30035  -8.75887  H
 N-NC--0.761500        0    -2.2261   -5.02015  -7.92042  H
 C-CQ-0.587500         0    -1.3808   -5.12606  -6.88361  H
 N-NC--0.699700        0    -1.62375  -5.54634  -5.6414   H
 C-CB-0.305300         0    -2.88339  -5.985    -5.52244  H
 H-H1-0.067900         0    -5.1047   -9.27871  -1.16055  L
 H-H1-0.067900         0    -6.085    -8.10276  -0.26986  L
 H-H1-0.117400         0    -3.77662  -7.29337  -0.32832  H
 H-H1-0.061500         0    -5.52693  -5.83239  -2.31439  H
 H-HO-0.437600         0    -6.10988  -5.2645   -0.21451  H
 H-H1-0.097200         0    -3.92008  -4.44096  -3.00561  H
 H-HO-0.418600         0    -0.69513  -5.49642  -0.39521  H
 H-H2-0.200700         0    -1.96457  -6.44442  -3.0188   H
 H-H5-0.155300         0    -5.48411  -7.27756  -4.13953  H
 H-H-0.411500          0    -4.16519  -4.62966  -9.48577  H
 H-H-0.411500          0    -5.36969  -5.32814  -8.49444  H
 H-H5-0.047300         0    -0.36783  -4.79013  -7.07267  H
 C-CQ-0.587500         0     6.66814   1.81656  -3.06473  L
 P-P-1.166200          0     0.81839  -2.85654   1.3464   H
 N-N3-0.001700         0    -3.71307  -2.9883    0.63251  H
 C-CT-0.058800         0    -3.45592  -2.53822  -0.74576  H
 C-CT-0.090900         0    -3.19625  -1.02759  -0.72862  H
 C-CT--0.023600        0    -2.79883  -0.3426   -2.05211  H
 C-C-0.808700          0    -3.24724   1.11686  -2.013    H
 O-O2--0.818900        0    -2.52665   1.94683  -1.4219   H
 O-O2--0.818900        0    -4.38644   1.38162  -2.55471  H
 C-C-0.562100          0    -2.32068  -3.3183   -1.37968  H
 O-O--0.588900         0    -1.26593  -2.83646  -1.70083  H
 O-OS--0.421000        0    -0.65357  -2.94622   0.9967   H
 O-O2--0.776000        0     1.68552  -3.9076    0.5269   H
 O-O2--0.776000        0     1.14648  -2.96816   2.83682  H
 O-OS--0.498900        0     1.44192  -1.47311   0.8179   H
 C-CT-0.055800         0     1.21681  -0.33941   1.64801  H
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 C-CT-0.106500        0     1.39665   0.94027   0.82033  L    H-H1
1776  0.        0.
 O-OS--0.354800       0     2.75536   1.15751   0.45016  L
 C-CT-0.039400        0     2.89542   1.10113  -0.9692   L
 N-N*--0.025100       0     4.02798   0.19797  -1.30732  L
 C-CB-0.305300        0     5.17438   0.5597   -1.98277  L
 N-NC--0.699700       0     5.43829   1.75736  -2.56998  L
 N-NC--0.761500       0     7.61394   0.88268  -3.04186  L
 C-CA-0.700900        0     7.30366  -0.28966  -2.4853   L
 N-N2--0.901900       0     8.28863  -1.17261  -2.505    L
 C-CB-0.051500        0     6.02905  -0.50851  -1.90252  L
 N-NB--0.607300       0     5.42294  -1.57848  -1.2332   L
 C-CK-0.200600        0     4.24277  -1.10362  -0.9143   L
 C-CT-0.067000        0     1.54854   0.68075  -1.56555  L
 O-OH--0.613900       0     1.28238   1.382    -2.77624  L
 C-CT-0.202200        0     0.53446   0.97414  -0.44357  L
 O-OH--0.654100       0    -0.08097   2.2557   -0.49706  L
 H-H5-0.047300        0     6.93493   2.75023  -3.53985  L
 H-H-0.239100         0    -2.97919  -2.6164    1.24544  H
 H-H-0.239100         0    -3.67423  -4.00357   0.7072   H
 H-H-0.239100         0    -5.31997  -2.44488   0.80088  H
 H-HP-0.120200        0    -4.36471  -2.76203  -1.32287  H
 H-HC--0.023200       0    -2.39052  -0.83025  -0.01841  H
 H-HC--0.023200       0    -4.12572  -0.59415  -0.34813  H
 H-HC--0.031500       0    -3.24243  -0.84267  -2.91421  H
 H-HC--0.031500       0    -1.71556  -0.37809  -2.16348  H
 H-H1-0.067900        0     1.91778  -0.34185   2.4874   H
 H-H1-0.067900        0     0.19143  -0.34522   2.04228  H
 H-H1-0.117400        0     1.0846    1.76676   1.45598  L
 H-H2-0.200700        0     3.12291   2.09788  -1.35648  L
 H-H-0.411500         0     8.13221  -2.11003  -2.15877  L
 H-H-0.411500         0     9.16553  -0.90338  -2.93213  L
 H-H5-0.155300        0     3.50445  -1.68023  -0.37186  L
 H-H1-0.097200        0     1.54877  -0.39419  -1.74248  L
 H-HO-0.418600        0     1.80401   0.97373  -3.51736  L
 H-H1-0.061500        0    -0.2319    0.19833  -0.41468  L
 H-HO-0.437600        0    -0.94331   2.13915  -0.96281  L
 O-OW--0.834000       0     6.22755   3.7662   -0.40747  L
 H-HW-0.417000        0     5.277     3.87083  -0.22496  L
 H-HW-0.417000        0     6.47376   3.09131   0.24962  L
 O-OW--0.834000       0     11.60195   11.1351  -1.27481  L
 H-HW-0.417000        0     12.28665   10.98241  -0.60086  L
 H-HW-0.417000        0     12.10687   11.49797  -2.02236  L
 O-OW--0.834000       0     10.45945   8.72064  -1.14875  L
 H-HW-0.417000        0     10.69121   9.67451  -1.16305  L
 H-HW-0.417000        0     11.33527   8.29841  -1.04783  L
 O-OW--0.834000       0     8.21397   7.24734  -11.83865  L
 H-HW-0.417000        0     7.52415   7.55483  -12.42591  L
 H-HW-0.417000        0     7.83083   6.41298  -11.47204  L
 O-OW--0.834000       0     17.84536  -8.18124   0.23864  L
 H-HW-0.417000        0     18.68077  -8.59397   0.47349  L
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H-HW-0.417000        0     17.23432  -8.53631   0.91048  L
O-OW--0.834000       0     17.48675  -6.43962  -1.88601  L
H-HW-0.417000        0     17.55854  -7.12135  -1.18807  L
H-HW-0.417000        0     18.02308  -5.72617  -1.53167  L
O-OW--0.834000       0     10.29952   2.52012  -10.15849  L
H-HW-0.417000        0     9.42341   2.81851  -9.82841  L
H-HW-0.417000        0     10.49293   3.1989   -10.81785  L
O-OW--0.834000       0     6.38007  -7.74481  -3.62942  L
H-HW-0.417000        0     5.53586  -8.22356  -3.65941  L
H-HW-0.417000        0     6.1258   -6.84998  -3.94567  L
O-OW--0.834000       0     2.14804  -4.28708  -5.31398  L
H-HW-0.417000        0     2.01863  -4.14945  -6.27451  L
H-HW-0.417000        0     2.34413  -3.37603  -5.00105  L
O-OW--0.834000       0     9.97569   5.09082  -11.37294  L
H-HW-0.417000        0     9.07611   4.8167   -11.09296  L
H-HW-0.417000        0     9.7807    5.93868  -11.79795  L
O-OW--0.834000       0     0.41411  -8.29032  -7.91462  L
H-HW-0.417000        0     0.49188  -8.97539  -8.58213  L
H-HW-0.417000        0     0.04471  -8.79293  -7.15921  L
O-OW--0.834000       0    -0.025    -7.36879  -4.11391  L
H-HW-0.417000        0    -0.59088  -6.90327  -4.747    L
H-HW-0.417000        0     0.03458  -8.27854  -4.53533  L
O-OW--0.834000       0     3.90818  -8.97613  -3.8      L
H-HW-0.417000        0     3.17123  -9.53353  -3.47662  L
H-HW-0.417000        0     3.47746  -8.09389  -3.86427  L
O-OW--0.834000       0     0.05826  -4.51323  -3.60647  L
H-HW-0.417000        0     0.88395  -4.45542  -4.12181  L
H-HW-0.417000        0    -0.55052  -4.93256  -4.23279  L
O-OW--0.834000       0     0.13635  -5.58569  -0.91767  H
H-HW-0.417000        0    -0.07272  -5.09679  -1.74241  H
H-HW-0.417000        0     1.10741  -4.50786  -0.01528  H
O-OW--0.834000       0     5.56544  -5.41397  -4.65604  L
H-HW-0.417000        0     5.10151  -5.54391  -5.50238  L
H-HW-0.417000        0     5.33194  -4.49938  -4.4075   L
O-OW--0.834000       0    -6.47239  -8.76856   2.13222  L
H-HW-0.417000        0    -6.30337  -7.9534    2.647    L
H-HW-0.417000        0    -7.06995  -8.45914   1.43791  L
O-OW--0.834000       0     5.07656  -10.51988  -1.61231  L
H-HW-0.417000        0     4.25554  -10.31662  -1.13397  L
H-HW-0.417000        0     4.9403   -10.08372  -2.46491  L
O-OW--0.834000       0     2.54477  -6.67795  -3.9406   L
H-HW-0.417000        0     1.58756  -6.89482  -3.99586  L
H-HW-0.417000        0     2.59241  -5.81978  -4.40292  L
O-OW--0.834000       0     4.74626  -6.55974  -0.12703  L
H-HW-0.417000        0     3.90352  -6.9931   -0.3538   L
H-HW-0.417000        0     4.67564  -5.74792  -0.68088  L
O-OW--0.834000       0     4.36836  -6.22612  -7.00717  L
H-HW-0.417000        0     4.21525  -7.18309  -6.87478  L
H-HW-0.417000        0     3.49752  -5.89593  -7.2515   L
O-OW--0.834000       0     2.99251  -7.43081   4.89335  L
H-HW-0.417000        0     2.72936  -6.5188    4.69838  L
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H-HW-0.417000        0     2.99767  -7.46376   5.86174  L
O-OW--0.834000       0     4.86421  -2.93782  -3.71116  L
H-HW-0.417000        0     4.0281   -2.4996   -3.97495  L
H-HW-0.417000        0     5.11289  -2.45289  -2.90524  L
O-OW--0.834000       0     0.74869  -13.95786  -3.33394  L
H-HW-0.417000        0    -0.12919  -13.73069  -3.69865  L
H-HW-0.417000        0     1.34801  -13.61339  -4.01951  L
O-OW--0.834000       0     4.01358  -4.48259  -1.56837  L
H-HW-0.417000        0     4.40799  -4.18475  -2.4018   L
H-HW-0.417000        0     3.19408  -3.94844  -1.53021  L
O-OW--0.834000       0     2.69945  -9.71169  -0.45414  L
H-HW-0.417000        0     2.24954  -10.19282  -1.17238  L
H-HW-0.417000        0     2.5025   -8.77917  -0.69281  L
O-OW--0.834000       0     0.14446  -11.18439  -7.58872  L
H-HW-0.417000        0     0.04521  -10.73028  -6.69561  L
H-HW-0.417000        0    -0.65378  -11.71379  -7.61571  L
O-OW--0.834000       0     7.50857  -10.62791  -0.40325  L
H-HW-0.417000        0     7.32538  -9.67453  -0.40417  L
H-HW-0.417000        0     6.73323  -10.96513  -0.8889   L
O-OW--0.834000       0     4.02007  -4.4545    1.62136  L
H-HW-0.417000        0     4.21724  -5.28117   1.15335  L
H-HW-0.417000        0     3.17797  -4.1803    1.1971   L
O-OW--0.834000       0     1.89551  -2.83634  -2.09673  H
H-HW-0.417000        0     0.93271  -2.98419  -2.06646  H
H-HW-0.417000        0     2.00539  -2.41479  -2.98479  H
O-OW--0.834000       0     8.95717  -8.13116  -4.17757  L
H-HW-0.417000        0     7.99874  -8.0666   -3.9684   L
H-HW-0.417000        0     9.21806  -7.19378  -4.25108  L
O-OW--0.834000       0     4.31806  -8.94751  -6.57506  L
H-HW-0.417000        0     3.80357  -9.6962   -6.93964  L
H-HW-0.417000        0     4.27157  -9.10167  -5.61497  L
O-OW--0.834000       0     1.68568  -3.80873  -7.95814  L
H-HW-0.417000        0     1.3813   -2.88651  -8.07606  L
H-HW-0.417000        0     1.49294  -4.21194  -8.80732  L
O-OW--0.834000       0     2.68781  -1.38079   4.59422  H
H-HW-0.417000        0     1.95432  -1.79716   4.10764  H
H-HW-0.417000        0     3.34162  -2.1075    4.54627  H
O-OW--0.834000       0     2.00678  -12.31524  -5.12789  L
H-HW-0.417000        0     2.36218  -12.07223  -5.99603  L
H-HW-0.417000        0     1.1192   -11.86806  -5.12423  L
O-OW--0.834000       0     6.68795  -7.78676  -7.63265  L
H-HW-0.417000        0     6.16901  -6.97552  -7.5259   L
H-HW-0.417000        0     6.07273  -8.45442  -7.28742  L
O-OW--0.834000       0     2.32633  -7.19733  -1.26353  L
H-HW-0.417000        0     1.62542  -6.55462  -1.04251  L
H-HW-0.417000        0     2.53877  -6.94815  -2.18462  L
O-OW--0.834000       0     1.85824  -10.55286  -2.99753  L
H-HW-0.417000        0     2.09603  -11.41226  -3.38679  L
H-HW-0.417000        0     1.12122  -10.28002  -3.60177  L
O-OW--0.834000       0    -7.86555  -5.54316   0.11243  L
H-HW-0.417000        0    -8.39481  -4.92453   0.64707  L
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H-HW-0.417000        0    -8.27054  -6.40212   0.31513  L
O-OW--0.834000       0     2.81355  -11.06042  -7.51915  L
H-HW-0.417000        0     3.03325  -11.57427  -8.30131  L
H-HW-0.417000        0     1.83085  -11.00637  -7.56741  L
O-OW--0.834000       0    -3.63826  -3.12773  -13.10575  L
H-HW-0.417000        0    -3.21509  -3.9922   -13.07349  L
H-HW-0.417000        0    -3.81176  -2.95261  -12.16096  L
O-OW--0.834000       0     9.27488  -8.05363  -8.39762  L
H-HW-0.417000        0     9.06471  -8.42967  -9.25544  L
H-HW-0.417000        0     8.38197  -7.91504  -8.01111  L
O-OW--0.834000       0     2.07546  -6.90139   2.10417  H
H-HW-0.417000        0     2.013    -6.21001   2.84642  H
H-HW-0.417000        0     1.28157  -7.45223   2.30006  H
O-OW--0.834000       0    -0.48009  -8.31404  -0.00717  L
H-HW-0.417000        0    -0.15795  -7.45765  -0.32548  L
H-HW-0.417000        0    -0.64022  -8.79692  -0.8353   L
O-OW--0.834000       0     4.18145  -3.67616   4.22882  L
H-HW-0.417000        0     4.33153  -3.80299   3.2699   L
H-HW-0.417000        0     3.41536  -4.25343   4.3711   L
O-OW--0.834000       0     1.7756   -5.13343   4.00345  H
H-HW-0.417000        0     1.47349  -4.29417   3.50426  H
H-HW-0.417000        0     0.91298  -5.45992   4.38381  H
O-OW--0.834000       0    -0.92622  -9.40505  -2.57224  L
H-HW-0.417000        0    -0.70866  -8.5018   -2.86126  L
H-HW-0.417000        0    -0.81875  -9.875    -3.44677  L
C-CW--0.220700       0     8.04816  -10.46408   10.4482  L
H-H4-0.186200        0     9.06945  -10.38691   10.09914  L
C-CT--0.149000       0     12.25636  -3.65869   12.96532  L
H-H1-0.097600        0     12.2146  -2.83723   13.6826  L
H-H1-0.097600        0     11.71316  -4.51628   13.36279  L
H-H1-0.097600        0     13.30218  -3.93311   12.81306  L
H-HC                 0    -6.87308  -10.15573  -7.42016  L
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**TS2**

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N-N--0.347900        0    -7.40325   15.27109   3.84399  L
 C-CT--0.263700       -1   -7.33662   13.90735   4.38986  L
 C-C-0.734100          0    -6.5305    13.03018   3.43492  L
 O-O--0.589400         0    -6.91183   12.90092   2.27815  L
 C-CT--0.000700        0    -8.76136   13.32751   4.55412  L
 C-CT-0.039000         0    -9.53791   13.91421   5.74433  L
 C-CT-0.048600         0    -10.96844   13.34945   5.86579  L
 N-N2--0.529502        0    -11.03237   11.94483   6.33458  L
 C-CA-0.807600         0    -10.94882   11.50186   7.5781   L
 N-N2--0.862702        0    -10.64518   12.27581   8.5828   L
 N-N2--0.862702        0    -11.18378   10.25078   7.83547  L
 H-H-0.274700          0    -7.19155   15.3944   2.85346  L
 H-H-0.274700          0    -7.43642   16.08595   4.44452  L
 H-H1-0.156001         0    -6.83062   13.91596   5.35563  L
 H-HC-0.032700         0    -8.69522   12.24742   4.68162  L
 H-HC-0.032700         0    -9.32572   13.51317   3.64112  L
 H-HC-0.028500         0    -9.61376   14.99377   5.60806  L
 H-HC-0.028500         0    -8.98915   13.72733   6.66774  L
 H-H1-0.068701         0    -11.46075   13.42522   4.89395  L
 H-H1-0.068701         0    -11.53189   13.98     6.55708  L
 H-H-0.345600          0    -11.32502   11.23026   5.67664  L
 H-H-0.447800          0    -10.60903   11.90826   9.51591  L
 H-H-0.447800          0    -10.50445   13.25396   8.41458  L
 H-H-0.447800          0    -11.15198   9.8778    8.76451  L
 H-H-0.447800          0    -11.50305   9.66856   7.06251  L
 N-N--0.415700         0    -5.45438   12.42625   3.93442  L
 C-CT--0.087500       -1   -4.48506   11.63422   3.16311  L
 C-C-0.597300          0    -4.36284   10.23062   3.73674  L
 O-O--0.567900         0    -4.33072   10.07884   4.96006  L
 C-CT-0.298500         0    -3.14552   12.3869   3.05021  L
 C-CT--0.319200        0    -2.48022   12.62983   4.40674  L
 C-CT--0.319200        0    -2.17869   11.66899   2.10713  L
 H-H-0.271900          0    -5.24137   12.55113   4.91068  L
 H-H1-0.096900         0    -4.8697    11.51973   2.15148  L
 H-HC--0.029700        0    -3.35193   13.36536   2.61532  L
 H-HC-0.079100         0    -3.13864   13.18978   5.0675   L
 H-HC-0.079100         0    -1.5708    13.21516   4.26207  L
 H-HC-0.079100         0    -2.21142   11.68345   4.87417  L
 H-HC-0.079100         0    -1.25534   12.24393   2.02472  L
 H-HC-0.079100         0    -2.62586   11.58845   1.11702  L
 H-HC-0.079100         0    -1.94156   10.67457   2.47784  L
 N-N--0.347900         0    -4.37893   9.20303   2.87287  L
 C-CT--0.263700       -1   -4.5729    7.81262   3.31803  L
 C-C-0.734100          0    -3.42228   6.84475   3.11366  L
 O-O--0.589400         0    -2.50563   7.09316   2.34206  L
 C-CT--0.000700        0    -5.94856   7.23583   2.91568  L
 C-CT-0.039000         0    -6.01439   6.16183   1.81305  L    H-H1
48    0.        0.
 C-CT-0.048600         0    -5.37816   6.56739   0.48154  H
 N-N2--0.529500        0    -5.66536   5.60691  -0.57324  H
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 C-CA-0.807600         0    -4.99054   4.45943  -0.80451  H
 N-N2--0.862700        0    -3.70594   4.32487  -0.45099  H
 N-N2--0.862700        0    -5.63122   3.44581  -1.36556  H
 H-H-0.274700          0    -4.37447   9.42324   1.88418  L
 H-H1-0.156000         0    -4.62519   7.8552    4.40634  L
 H-HC-0.032700         0    -6.60755   8.05395   2.65559  L
 H-HC-0.032700         0    -6.38243   6.77763   3.80618  L
 H-HC-0.028500         0    -7.06778   5.94602   1.63636  L
 H-HC-0.028500         0    -5.55351   5.23764   2.16169  L
 H-H1-0.068700         0    -4.30191   6.67367   0.59599  H
 H-H1-0.068700         0    -5.77739   7.53152   0.18417  H
 H-H-0.345600          0    -6.65273   5.50422  -0.83637  H
 H-H-0.447800          0    -3.22128   3.48006  -0.8072   H
 H-H-0.447800          0    -3.15489   5.18503  -0.40106  H
 H-H-0.447800          0    -5.14642   2.61678  -1.81313  H
 H-H-0.447800          0    -6.636     3.63033  -1.51711  H
 N-N--0.415700         0    -3.50489   5.72187   3.81435  L
 C-CT--0.002400       -1    -2.58394   4.60454   3.74348  L
 C-C-0.597300          0    -3.29244   3.28228   4.0584   L
 O-O--0.567900         0    -4.07809   3.20572   5.00312  L
 C-CT--0.034300        0    -1.43636   4.89582   4.72887  L
 C-CA-0.011800         0    -0.47182   3.75809   5.01438  L
 C-CA--0.125600        0     0.33968   3.22007   3.99755  L
 C-CA--0.125600        0    -0.36336   3.25638   6.32414  L
 C-CA--0.170400        0     1.24961   2.18728   4.29654  L
 C-CA--0.170400        0     0.53201   2.21319   6.61734  L
 C-CA--0.107200        0     1.34213   1.67806   5.60182  L
 H-H-0.271900          0    -4.22219   5.67201   4.52994  L
 H-H1-0.097800         0    -2.17111   4.54085   2.73509  L
 H-HC-0.029500         0    -1.87547   5.21629   5.67566  L
 H-HC-0.029500         0    -0.85804   5.73774   4.34537  L
 H-HA-0.133000         0     0.27253   3.60671   2.99164  L
 H-HA-0.133000         0    -0.98045   3.67079   7.10539  L
 H-HA-0.143000         0     1.90063   1.77912   3.53701  L
 H-HA-0.143000         0     0.58865   1.81657   7.61892  L
 H-HA-0.129700         0     2.03927   0.87713   5.81512  L
 N-N--0.415700         0    -3.01896   2.24975   3.25599  L
 C-CT-0.033700        -1    -3.81345   1.02218   3.20425  L
 C-C-0.597300          0    -2.96363  -0.27039   3.34271  L
 O-O--0.567900         0    -2.85425  -1.05278   2.3995   L
 C-CT--0.182500        0    -4.6399    1.10309   1.91426  L
 H-H-0.271900          0    -2.36747   2.39809   2.50127  L
 H-H1-0.082300         0    -4.52671   1.01412   4.02642  L
 H-HC-0.060300         0    -3.98273   1.2175    1.05221  L
 H-HC-0.060300         0    -5.31792   1.95682   1.95845  L
 H-HC-0.060300         0    -5.23038   0.19958   1.79888  L
 N-N--0.254800         0    -2.33383  -0.55196   4.49713  L
 C-CT--0.026600        0    -1.55911  -1.77739   4.70871  L    H-H2
98    0.        0.
 C-C-0.589600          0    -2.41734  -3.06784   4.60558  H
 O-O--0.574800         0    -3.38819  -3.31753   5.30199  H
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 C-CT--0.007000       0    -0.90293  -1.6229    6.08674  L
 C-CT-0.018900        0    -1.77196  -0.58004   6.78648  L
 C-CT-0.019200        0    -2.18572   0.32927   5.63808  L
 H-H1-0.064100        0    -0.7656   -1.82101   3.96203  L
 H-HC-0.025300        0     0.10832  -1.231     5.96492  L
 H-HC-0.025300        0    -0.87961  -2.56182   6.64143  L
 H-HC-0.021300        0    -1.22965  -0.03917   7.56141  L
 H-HC-0.021300        0    -2.65806  -1.06281   7.19373  L
 H-H1-0.039100        0    -3.09172   0.87702   5.88313  L
 H-H1-0.039100        0    -1.39028   1.03135   5.41288  L
 N-N--0.415700        0    -1.94184  -3.92326   3.66125  H
 C-CT--0.024900       0    -2.38656  -5.29523   3.51988  H
 C-C-0.597300         0    -1.93152  -6.10842   4.74412  L    H-H1
111   0.        0.
 O-O--0.567900        0    -0.73628  -6.10443   5.04411  L
 C-CT-0.211700        0    -1.75265  -5.94469   2.2921   H
 O-OH--0.654600       0    -2.02264  -5.27633   1.07462  H
 H-H-0.271900         0    -1.208    -3.60578   3.03437  H
 H-H1-0.084300        0    -3.47444  -5.31804   3.43336  H
 H-H1-0.035200        0    -2.1441   -6.9615    2.20357  H
 H-H1-0.035200        0    -0.66083  -6.01344   2.43469  H
 H-HO-0.427500        0    -1.52882  -4.41626   1.14746  H
 N-N--0.254800        0    -2.82354  -6.80418   5.47123  L
 C-CT--0.026600       0    -2.47691  -7.64463   6.6124   L
 C-C-0.589600         0    -1.91731  -8.98689   6.11685  L
 O-O--0.574800        0    -2.46963  -10.05273   6.37167  L
 C-CT--0.007000       0    -3.78341  -7.78387   7.39786  L
 C-CT-0.018900        0    -4.84009  -7.78632   6.29916  L
 C-CT-0.019200        0    -4.24772  -6.87464   5.22801  L
 H-H1-0.064100        0    -1.73108  -7.1527    7.23632  L
 H-HC-0.025300        0    -3.91714  -6.90417   8.02305  L
 H-HC-0.025300        0    -3.82517  -8.68377   8.01242  L
 H-HC-0.021300        0    -5.78168  -7.38869   6.66742  L
 H-HC-0.021300        0    -4.96765  -8.79405   5.90082  L
 H-H1-0.039100        0    -4.43634  -7.29332   4.23942  L
 H-H1-0.039100        0    -4.67509  -5.87792   5.31766  L
 N-N--0.415700        0    -0.79844  -8.91694   5.4031   L
 C-CT--0.038900      -1    -0.18401  -10.01041   4.65117  L
 C-C-0.597300         0     1.3397   -10.01617   4.8896   L
 O-O--0.567900        0     2.14502  -9.75493   3.99483  L
 C-CT-0.365400        0    -0.519    -9.91997   3.14721  L
 O-OH--0.676100       0    -0.26676  -8.62211   2.65223  L
 C-CT--0.243800       0    -1.9884   -10.22275   2.85355  L
 H-H-0.271900         0    -0.43943  -7.98963   5.21204  L
 H-H1-0.100700        0    -0.56249  -10.96867   5.01114  L
 H-H1-0.004300        0     0.09318  -10.63955   2.60204  L
 H-HC-0.064200        0    -2.632    -9.47666   3.31883  L
 H-HC-0.064200        0    -2.24414  -11.20823   3.24175  L
 H-HC-0.064200        0    -2.15459  -10.21474   1.77612  L
 H-HO-0.410200        0    -0.29674  -8.67837   1.676    L
 N-N--0.415700        0     1.75976  -10.29104   6.12959  L
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C-CT--0.025200       -1    3.16912  -10.3655   6.5461   L
C-C-0.597300         0     3.75326  -9.07469   7.15985  L
O-O--0.567900        0     3.15155  -7.9997    7.09573  L
H-H-0.271900         0     1.05477  -10.50129   6.82248  L
H-H1-0.069800        0     3.78141  -10.62125   5.68088  L
H-H1-0.069800        0     3.28378  -11.17661   7.25999  L
N-N--0.415700        0     4.95127  -9.18972   7.75233  L
C-CT--0.058100       -1    5.69762  -8.13509   8.47452  L
C-C-0.597300         0     5.93274  -6.86798   7.63295  L
O-O--0.567900        0     6.25668  -6.94695   6.44886  L
C-CT--0.007400       0     7.04193  -8.69962   8.9608   L
C-CC-0.186800        0     6.93542  -9.80676   9.98336  L
N-NB--0.543200       0     5.76153  -10.25166   10.59552  L
C-CR-0.163500        0     6.13701  -11.20685   11.45988  L
N-NA--0.279500       0     7.46902  -11.38726   11.41188  L
H-H-0.271900         0     5.35547  -10.11307   7.78178  L
H-H1-0.136000        0     5.11392  -7.85186   9.35051  L
H-HC-0.036700        0     7.61674  -7.88996   9.4124   L
H-HC-0.036700        0     7.60547  -9.0681    8.1021   L
H-H-0.333900         0     7.9902   -12.04581   11.97704  L
H-H5-0.143500        0     5.46237  -11.74981   12.10993  L
N-N--0.415700        0     5.80296  -5.70393   8.28043  L
C-CT--0.051800       0     6.01511  -4.36427   7.7179   L
C-C-0.597300         0     7.4362   -4.18716   7.1607   L
O-O--0.567900        0     8.40361  -4.27452   7.92258  L
C-CT--0.110200       0     5.76005  -3.33812   8.84066  L
C-CT-0.353100        0     6.00452  -1.86568   8.45178  L
C-CT--0.412100       0     4.95732  -1.31936   7.48324  L
C-CT--0.412100       0     5.98939  -1.00688   9.71439  L
H-H-0.271900         0     5.56632  -5.75494   9.25632  L
H-H1-0.092200        0     5.29729  -4.20367   6.91339  L
H-HC-0.045700        0     6.42694  -3.58121   9.66999  L
H-HC-0.045700        0     4.74072  -3.44648   9.1998   L
H-HC--0.036100       0     6.98319  -1.76097   7.99198  L
H-HC-0.100000        0     3.9667   -1.35688   7.92613  L
H-HC-0.100000        0     4.96617  -1.89849   6.56087  L
H-HC-0.100000        0     5.18373  -0.28531   7.23665  L
H-HC-0.100000        0     5.02027  -1.08561   10.20466  L
H-HC-0.100000        0     6.18819   0.03141   9.45521  L
H-HC-0.100000        0     6.76689  -1.34648   10.39884  L
N-N--0.415700        0     7.56129  -3.83466   5.87804  L
C-CT--0.058100       -1    8.84403  -3.47875   5.25569  L
C-C-0.597300         0     8.97385  -1.97512   5.00671  L
O-O--0.567900        0     8.00038  -1.21634   5.0319   L
C-CT--0.007400       0     9.1038   -4.33546   4.00378  L
C-CC-0.186800        0     8.55918  -3.7706    2.72086  L
N-NB--0.543200       0     9.25341  -2.91097   1.87021  L
C-CW--0.220700       0     7.34159  -4.05038   2.18233  L
C-CR-0.163500        0     8.43614  -2.70667   0.82601  L
N-NA--0.279500       0     7.27359  -3.35407   0.99587  L
H-H-0.271900         0     6.7116   -3.72831   5.33054  L
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H-H1-0.136000        0     9.64153  -3.72873   5.9536   L
H-HC-0.036700        0     8.70656  -5.34022   4.15607  L
H-HC-0.036700        0     10.17965  -4.43661   3.87028  L
H-H4-0.186200        0     6.58711  -4.70027   2.60059  L
H-H-0.333900         0     6.4985   -3.33568   0.3344   L
H-H5-0.143500        0     8.68433  -2.12495  -0.04965  L
N-N--0.415700        0     10.21363  -1.5389    4.80154  L
C-CT--0.087500       -1    10.59869  -0.12787   4.66395  L
C-C-0.597300         0     9.85364   0.63439   3.56844  L
O-O--0.567900        0     9.52465   1.79535   3.78205  L
C-CT-0.298500        0     12.12349   0.01746   4.49896  L
C-CT--0.319200       0     12.84306  -0.36468   5.79823  L
C-CT--0.319200       0     12.69003  -0.82891   3.35366  L
H-H-0.271900         0     10.94818  -2.23925   4.80809  L
H-H1-0.096900        0     10.33303   0.37315   5.5937   L
H-HC--0.029700       0     12.34706   1.06223   4.2904   L
H-HC-0.079100        0     12.67892  -1.41625   6.0369   L
H-HC-0.079100        0     12.48039   0.25012   6.62118  L
H-HC-0.079100        0     13.91426  -0.19684   5.68741  L
H-HC-0.079100        0     12.50442  -1.88908   3.52533  L
H-HC-0.079100        0     13.76602  -0.6853    3.28893  L
H-HC-0.079100        0     12.24878  -0.52607   2.40609  L
N-N--0.415700        0     9.54961   0.02118   2.42174  L
C-CT--0.025200       -1    8.75426   0.64712   1.35851  L
C-C-0.597300         0     7.31612   0.94692   1.79393  L
O-O--0.567900        0     6.83741   2.06225   1.59103  L
H-H-0.271900         0     9.78459  -0.96364   2.34052  L
H-H1-0.069800        0     8.72699   0.00501   0.48062  L
H-H1-0.069800        0     9.21876   1.58841   1.07576  L
N-N--0.415700        0     6.64165  -0.01587   2.42836  L
C-CT--0.025200       0     5.33419   0.17609   3.06661  L
C-C-0.597300         0     5.34758   1.2908    4.12162  L
O-O--0.567900        0     4.57492   2.24771   4.04697  L
H-H-0.271900         0     7.10236  -0.90783   2.5579   L
H-H1-0.069800        0     5.04069  -0.75403   3.54959  L
H-H1-0.069800        0     4.59153   0.42093   2.30779  L
N-N--0.415700        0     6.26307   1.20181   5.09159  L
C-CT-0.033700        -1    6.47053   2.2145    6.13458  L
C-C-0.597300         0     6.78114   3.60837   5.57174  L
O-O--0.567900        0     6.30099   4.60746   6.10146  L
C-CT--0.182500       0     7.57693   1.72756   7.06097  L
H-H-0.271900         0     6.85845   0.37779   5.08248  L
H-H1-0.082300        0     5.54623   2.29603   6.70533  L
H-HC-0.060300        0     7.29669   0.74484   7.42698  L
H-HC-0.060300        0     7.68977   2.41356   7.90121  L
H-HC-0.060300        0     8.521     1.65778   6.51936  L
N-N--0.347900        0     7.56833   3.69323   4.49582  L
C-CT--0.263700       -1    7.82803   4.92904   3.75342  L
C-C-0.734100         0     6.54847   5.58174   3.2177   L
O-O--0.589400        0     6.46816   6.80056   3.28638  L
C-CT--0.000700       0     8.943     4.68446   2.72168  L
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C-CT-0.039000        0     9.24254   5.83693   1.74501  L
C-CT-0.048600        0     8.3133    5.72124   0.53592  L
N-N2--0.529500       0     8.77542   6.46705  -0.63673  L
C-CA-0.807600        0     8.64554   6.06986  -1.88632  L
N-N2--0.862700       0     7.94619   5.03359  -2.23636  L
N-N2--0.862700       0     9.24311   6.71402  -2.83616  L
H-H-0.274700         0     7.99489   2.83339   4.16136  L
H-H1-0.156000        0     8.22367   5.65328   4.46398  L
H-HC-0.032700        0     8.7257    3.77894   2.15693  L
H-HC-0.032700        0     9.85567   4.48402   3.28086  L
H-HC-0.028500        0     10.27194   5.73004   1.39958  L
H-HC-0.028500        0     9.13238   6.80688   2.23178  L
H-H1-0.068700        0     7.30396   6.04231   0.79211  L
H-H1-0.068700        0     8.30068   4.66807   0.26602  L
H-H-0.345600         0     9.31305   7.31995  -0.51498  L
H-H-0.447800         0     7.9361    4.7792   -3.21601  L
H-H-0.447800         0     7.34732   4.56598  -1.55863  L
H-H-0.447800         0     9.23283   6.29986  -3.75826  L
H-H-0.447800         0     9.79059   7.52302  -2.56734  L
N-N--0.415700        0     5.54109   4.83471   2.75289  L
C-CT--0.038900      -1     4.20719   5.39785   2.42796  L
C-C-0.597300         0     3.57306   6.05979   3.65016  L
O-O--0.567900        0     3.11475   7.19231   3.5517   L
C-CT-0.365400        0     3.23901   4.34298   1.86859  L
O-OH--0.676100       0     3.85754   3.57644   0.86909  L
C-CT--0.243800       0     2.01011   4.96885   1.21118  L
H-H-0.271900         0     5.67242   3.83236   2.68856  L
H-H1-0.100700        0     4.33961   6.16826   1.66747  L
H-H1-0.004300        0     2.92308   3.67884   2.66984  L
H-HC-0.064200        0     1.43853   5.53521   1.94569  L
H-HC-0.064200        0     1.37544   4.18632   0.79474  L
H-HC-0.064200        0     2.32116   5.6393    0.40884  L
H-HO-0.410200        0     3.41258   2.71327   0.85727  L
N-N--0.415700        0     3.55913   5.38345   4.80676  L
C-CT-0.033700       -1     3.10055   5.9701    6.0714   L
C-C-0.597300         0     3.85486   7.25899   6.4194   L
O-O--0.567900        0     3.21875   8.27597   6.65092  L
C-CT--0.182500       0     3.15276   4.92607   7.18548  L
H-H-0.271900         0     3.95563   4.45259   4.81482  L
H-H1-0.082300        0     2.05569   6.25062   5.93814  L
H-HC-0.060300        0     2.59758   4.0411    6.88009  L
H-HC-0.060300        0     2.70249   5.34182   8.08727  L
H-HC-0.060300        0     4.18145   4.65153   7.3999   L
N-N--0.415700        0     5.19001   7.23092   6.42029  L
C-CT--0.051800      -1     6.05946   8.38996   6.64727  L
C-C-0.597300         0     5.7533    9.56072   5.71794  L
O-O--0.567900        0     5.57438   10.6799   6.18354  L
C-CT--0.110200       0     7.5257    7.92604   6.52753  L
C-CT-0.353100        0     8.57897   9.02175   6.78359  L
C-CT--0.412100       0     8.58808   9.47978   8.24179  L
C-CT--0.412100       0     9.97026   8.47917   6.44405  L
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H-H-0.271900          0      5.62046   6.33281   6.23022  L
H-H1-0.092200         0      5.88499   8.74107   7.66526  L
H-HC-0.045700         0      7.67726   7.54597   5.51928  L
H-HC-0.045700         0      7.69484   7.10339   7.22405  L
H-HC--0.036100        0      8.38794   9.87951   6.13989  L
H-HC-0.100000         0      9.36542   10.2294   8.38963  L
H-HC-0.100000         0      8.76812   8.63555   8.90676  L
H-HC-0.100000         0      7.63169   9.93689   8.4932   L
H-HC-0.100000         0      10.19576   7.61729   7.07203  L
H-HC-0.100000         0      10.71226   9.25877   6.61559  L
H-HC-0.100000         0      9.99939   8.18905   5.3938   L
N-N--0.415700         0      5.72307   9.30021   4.41462  L
C-CT--0.002400        -1     5.43739   10.29062   3.38799  L
C-C-0.597300          0      4.05419   10.92306   3.56795  L
O-O--0.567900         0      3.92251   12.14218   3.60123  L
C-CT--0.034300        0      5.60448   9.63912   2.00232  L
C-CA-0.011800         0      5.66837   10.60879   0.83497  L
C-CA--0.125600        0      6.91453   10.95938   0.27826  L
C-CA--0.125600        0      4.48879   11.1426   0.28161  L
C-CA--0.170400        0      6.98024   11.83977  -0.81682  L
C-CA--0.170400        0      4.55319   12.02421  -0.81216  L
C-CA--0.107200        0      5.79912   12.37463  -1.36067  L
H-H-0.271900          0      5.88872   8.3465    4.11541  L
H-H1-0.097800         0      6.16716   11.09696   3.47432  L
H-HC-0.029500         0      4.79075   8.93225   1.83155  L
H-HC-0.029500         0      6.53227   9.06648   2.00062  L
H-HA-0.133000         0      7.82832   10.55646   0.68946  L
H-HA-0.133000         0      3.52641   10.88276   0.69615  L
H-HA-0.143000         0      7.93976   12.11172  -1.2348   L
H-HA-0.143000         0      3.64245   12.43293  -1.22843  L
H-HA-0.129700         0      5.84667   13.05792  -2.19675  L
N-N--0.415700         0      3.02299   10.08885   3.69897  L
C-CT-0.014300         -1     1.64015   10.52729   3.84684  L
C-C-0.597300          0      1.33164   11.11146   5.25591  L
O-O--0.567900         0      0.32932   11.8025   5.41186  L
C-CT--0.204100        0      0.70142   9.36142   3.47199  L
C-C-0.713000          0      0.78169   8.9545    2.00307  L
O-O--0.593100         0      1.52399   9.48132   1.1953   L
N-N--0.919100         0     -0.00529   8.00388   1.56743  L
H-H-0.271900          0      3.20897   9.09463   3.63584  L
H-H1-0.104800         0      1.4634    11.34236   3.14149  L
H-HC-0.079700         0     -0.32324   9.65329   3.68852  L
H-HC-0.079700         0      0.94431   8.49632   4.0837   L
H-H-0.419600          0      0.10674   7.80319   0.59304  L
H-H-0.419600          0     -0.77495   7.61329   2.09689  L
N-N--0.415700         0      2.14013   10.83063   6.28742  L
C-CT--0.027500        -1     2.16048   11.51085   7.59965  L
C-C-0.597300          0      2.81114   12.90503   7.48753  L
N-N--0.415700         0      4.00926   12.98688   6.88905  L
C-CT--0.149000        -1     4.7966    14.20109   6.67567  L
O-O--0.567900         0      2.22482   13.88565   7.94251  L
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C-CT--0.005000       0     2.8896    10.62504   8.61914  L
C-C*--0.141500       0     3.21551   11.26102   9.93426  L
C-CW--0.163800       0     2.35784   11.44009   10.96416  L
C-CB-0.124300        0     4.49209   11.82517   10.36595  L
N-NA--0.341800       0     3.01846   12.06575   12.0066  L
C-CN-0.138000        0     4.33768   12.31943   11.6941  L
C-CA--0.238700       0     5.76154   11.97772   9.76587  L
C-CA--0.260100       0     5.3907    12.92058   12.39995  L
C-CA--0.197200       0     6.82696   12.58014   10.46328  L
C-CA--0.113400       0     6.64475   13.04839   11.77745  L
H-H-0.271900         0     2.86715   10.14597   6.1205   L
H-H-0.271900         0     4.39915   12.11945   6.53829  L
H-H1-0.112300        0     1.13876   11.66753   7.94289  L
H-HC-0.033900        0     3.83194   10.29521   8.18398  L
H-HC-0.033900        0     2.28422   9.73629   8.80238  L
H-H4-0.206200        0     1.31638   11.14605   10.95405  L
H-H-0.341200         0     2.58251   12.34001   12.87454  L
H-HA-0.170000        0     5.89934   11.64345   8.74798  L
H-HA-0.157200        0     5.23621   13.29086   13.40202  L
H-HA-0.144700        0     7.78762   12.69832   9.98163  L
H-HA-0.141700        0     7.46505   13.5197   12.30197  L
H-H1-0.097600        0     5.27653   14.49589   7.61017  L
H-H1-0.097600        0     4.14208   15.00828   6.34159  L
H-H1-0.097600        0     5.55546   14.01801   5.91394  L
N-N--0.415700        0    -3.71458   12.25514   8.4886   L
C-CT--0.002400      -1    -3.3515    10.88623   8.12442  L
C-C-0.597300         0    -4.46793   9.89564   8.47928  L
O-O--0.567900        0    -5.13977   10.05401   9.498    L
C-CT--0.034300       0    -2.03309   10.5409   8.83006  L
C-CA-0.011800        0    -1.47107   9.17286   8.49796  L
C-CA--0.125600       0    -0.92383   8.92869   7.225    L
C-CA--0.125600       0    -1.46334   8.15331   9.46907  L
C-CA--0.170400       0    -0.35966   7.67581   6.92974  L
C-CA--0.170400       0    -0.89177   6.90278   9.17514  L
C-CA--0.107200       0    -0.33649   6.66535   7.90594  L
H-H-0.271900         0    -4.39227   12.35044   9.23579  L
H-H-0.271900         0    -3.04023   12.99158   8.32045  L
H-H1-0.097800        0    -3.18188   10.84703   7.04865  L
H-HC-0.029500        0    -2.18067   10.61469   9.90893  L
H-HC-0.029500        0    -1.28395   11.28471   8.55251  L
H-HA-0.133000        0    -0.91481   9.71181   6.47996  L
H-HA-0.133000        0    -1.87775   8.33471   10.45078  L
H-HA-0.143000        0     0.07777   7.50004   5.9593   L
H-HA-0.143000        0    -0.86616   6.13408   9.93349  L
H-HA-0.129700        0     0.12189   5.71428   7.68238  L
N-N--0.415700        0    -4.68961   8.89952   7.6208   L
C-CT--0.059700      -1    -5.69993   7.84874   7.77602  L
C-C-0.597300         0    -5.04971   6.49183   7.49472  L
O-O--0.567900        0    -4.44402   6.32415   6.43641  L
C-CT-0.130300        0    -6.92603   8.09362   6.85846  L
C-CT--0.043000       0    -7.72315   9.37114   7.22118  L
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C-CT--0.320400       0    -7.89556   6.89865   6.95438  L
C-CT--0.066000       0    -7.23498   10.65726   6.54353  L
H-H-0.271900         0    -4.13181   8.88663   6.77468  L
H-H1-0.086900        0    -6.04805   7.83984   8.80962  L
H-HC-0.018700        0    -6.59302   8.16817   5.82261  L
H-HC-0.023600        0    -7.7259    9.50854   8.30329  L
H-HC-0.023600        0    -8.75807   9.24317   6.90522  L
H-HC-0.088200        0    -8.208     6.73843   7.98708  L
H-HC-0.088200        0    -7.43286   5.98706   6.57364  L
H-HC-0.088200        0    -8.77898   7.07414   6.34353  L
H-HC-0.018600        0    -6.23746   10.92953   6.87216  L
H-HC-0.018600        0    -7.90971   11.47043   6.80532  L
H-HC-0.018600        0    -7.22836   10.52596   5.4625   L
N-N--0.415700        -1   -5.19925   5.52424   8.41085  L
C-CT--0.051800       0    -4.61037   4.19132   8.27914  L
C-C-0.597300         0    -5.72685   3.1527    8.28378  L
O-O--0.567900        0    -6.44855   3.02277   9.27181  L
C-CT--0.110200       0    -3.5621    3.97714   9.38935  L
C-CT-0.353100        0    -2.74898   2.66904   9.25895  L
C-CT--0.412100       0    -1.39582   2.82344   9.96093  L
C-CT--0.412100       0    -3.43131   1.45045   9.88578  L
H-H-0.271900         0    -5.75312   5.7084    9.23359  L
H-H1-0.092200        0    -4.08898   4.1199    7.32438  L
H-HC-0.045700        0    -4.04392   4.01326   10.36772  L
H-HC-0.045700        0    -2.86992   4.81683   9.33197  L
H-HC--0.036100       0    -2.56464   2.45973   8.20597  L
H-HC-0.100000        0    -0.8137    1.9091    9.85008  L
H-HC-0.100000        0    -1.54983   3.02577   11.02164  L
H-HC-0.100000        0    -0.83759   3.64665   9.51739  L
H-HC-0.100000        0    -3.68943   1.65755   10.92473  L
H-HC-0.100000        0    -2.76362   0.59094   9.84738  L
H-HC-0.100000        0    -4.33727   1.19421   9.34193  L
N-N--0.347900        0    -5.84115   2.40356   7.18623  L
C-CT--0.263700       -1   -6.77576   1.28905   7.04076  L
C-C-0.734100         0    -6.02855  -0.03906   6.88821  L
O-O--0.589400        0    -5.19201  -0.17954   6.00465  L
C-CT--0.000700       0    -7.68845   1.51622   5.83107  L
C-CT-0.039000        0    -8.58642   0.28421   5.62908  L
C-CT-0.048600        0    -9.69973   0.53798   4.6359   L
N-N2--0.529500       0    -9.19285   0.73252   3.27061  L
C-CA-0.807600        0    -9.17851   1.83744   2.55801  L
N-N2--0.862700       0    -9.78538   2.93748   2.88684  L
N-N2--0.862700       0    -8.52359   1.83026   1.44465  L
H-H-0.274700         0    -5.21927   2.61133   6.40801  L
H-H1-0.156000        0    -7.40458   1.21806   7.93082  L
H-HC-0.032700        0    -7.08711   1.67959   4.93441  L
H-HC-0.032700        0    -8.30079   2.39905   6.00832  L
H-HC-0.028500        0    -9.04266   0.00656   6.58031  L
H-HC-0.028500        0    -7.99262  -0.54805   5.26018  L
H-H1-0.068700        0    -10.23183   1.41547   4.98583  L
H-H1-0.068700        0    -10.37319  -0.31855   4.65018  L
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 H-H-0.345600          0    -8.75898  -0.04784   2.78614  L
 H-H-0.447800          0    -9.7352    3.68444   2.19802  L
 H-H-0.447800          0    -10.56467   2.88465   3.54917  L
 H-H-0.447800          0    -8.53809   2.69097   0.89661  L
 H-H-0.447800          0    -8.1468    0.94253   1.12     L
 N-N--0.415700         0    -6.37669  -1.04115   7.68944  L
 C-CT--0.059700        -1   -5.97452  -2.43532   7.44453  L
 C-C-0.597300          0    -6.89328  -3.04539   6.3758   L
 O-O--0.567900         0    -8.10097  -2.82187   6.39812  L
 C-CT-0.130300         0    -6.12897  -3.24319   8.75541  L
 C-CT--0.043000        0    -5.36897  -2.64372   9.96276  L
 C-CT--0.320400        0    -5.72198  -4.71135   8.55171  L
 C-CT--0.066000        0    -3.88892  -2.3231    9.71949  L
 H-H-0.271900          0    -7.14588  -0.87628   8.32721  L
 H-H1-0.086900         0    -4.94075  -2.47512   7.10227  L
 H-HC-0.018700         0    -7.1868   -3.24335   9.02612  L
 H-HC-0.023600         0    -5.44006  -3.33572   10.80286  L
 H-HC-0.023600         0    -5.86672  -1.72306   10.27062  L
 H-HC-0.088200         0    -6.40657  -5.20284   7.85975  L
 H-HC-0.088200         0    -5.78662  -5.24598   9.49772  L
 H-HC-0.088200         0    -4.70847  -4.76397   8.15583  L
 H-HC-0.018600         0    -3.42076  -2.04154   10.66291  L
 H-HC-0.018600         0    -3.81031  -1.48493   9.03181  L
 H-HC-0.018600         0    -3.36611  -3.18331   9.30469  L
 N-N--0.516300         0    -6.36262  -3.85774   5.46513  L
 C-CT-0.039700         -1   -7.15273  -4.39564   4.34855  L
 C-C-0.536600          0    -7.26843  -5.92586   4.30358  L
 O-O--0.581900         0    -6.62945  -6.57726   3.47966  L
 C-CT-0.056000         0    -6.61555  -3.8024    3.01958  L    H-HC
485   0.        0.
 C-CT-0.013600         0    -6.81218  -2.27694   2.9225   H
 C-C-0.805400          0    -7.06679  -1.68232   1.54018  H
 O-O2--0.818800        0    -6.24092  -1.9413    0.53359  H
 O-O2--0.818800        0    -7.98571  -0.90616   1.36501  H
 H-H-0.293600          0    -5.3507   -3.91818   5.4413   L
 H-H1-0.110500         0    -8.18435  -4.0522    4.42149  L
 H-HC--0.017300        0    -7.15307  -4.26461   2.19893  L
 H-HC--0.017300        0    -5.55674  -4.03953   2.90199  L
 H-HC--0.042500        0    -5.938    -1.79642   3.37332  H
 H-HC--0.042500        0    -7.68991  -1.99362   3.50079  H
 N-N--0.516300         0    -8.10007  -6.52172   5.16491  L
 C-CT-0.038100         -1   -8.36362  -7.96638   5.21032  L
 C-C-0.536600          0    -9.5059   -8.41106   4.27651  L
 O-O--0.581900         0    -10.69076  -8.21102   4.5225   L
 C-CT--0.030300        0    -8.60025  -8.44964   6.65399  L
 C-C-0.799400          0    -9.81827  -7.83841   7.3447   L
 O-O2--0.801400        0    -9.98988  -6.60244   7.26246  L
 O-O2--0.801400        0    -10.54877  -8.58417   8.03545  L
 H-H-0.293600          0    -8.64133  -5.97644   5.82974  L
 H-H1-0.088000         0    -7.46087  -8.47809   4.87556  L
 H-HC--0.012200        0    -7.72383  -8.22548   7.25973  L
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H-HC--0.012200       0    -8.70917  -9.5356    6.63422  L
N-N--0.415700        0    -9.12383  -9.06223   3.18278  L
C-CT--0.038900       -1   -9.99378  -9.60118   2.11965  L
C-C-0.597300         0    -9.45252  -10.91382   1.53485  L
O-O--0.567900        0    -10.08392  -11.5187   0.66694  L
C-CT-0.365400        0    -10.13203  -8.57031   0.97787  L
O-OH--0.676100       0    -8.86533  -8.14832   0.51076  L
C-CT--0.243800       0    -10.8792  -7.30115   1.38584  L
H-H-0.271900         0    -8.12737  -9.05265   3.0055   L
H-H1-0.100700        0    -10.98386  -9.80526   2.52605  L
H-H1-0.004300        0    -10.6797  -9.02549   0.15184  L
H-HC-0.064200        0    -10.29422  -6.74041   2.11492  L
H-HC-0.064200        0    -11.84064  -7.56004   1.82822  L
H-HC-0.064200        0    -11.03738  -6.67075   0.51139  L
H-HO-0.410200        0    -8.67649  -8.68607  -0.30153  L
N-N--0.516300        0    -8.28866  -11.37065   2.00807  L
C-CT-0.038100        -1   -7.48484  -12.4546   1.44396  L
C-C-0.536600         0    -7.12993  -13.50851   2.52608  L
N-N--0.415700        0    -8.15688  -14.1452   3.10784  L
C-CT--0.149000       -1   -8.03274  -15.15561   4.1666   L
O-O--0.581900        0    -5.96748  -13.74887   2.85277  L
C-CT--0.030300       0    -6.25902  -11.82223   0.75626  L
C-C-0.799400         0    -5.64837  -12.73838  -0.29558  L
O-O2--0.801400       0    -4.41119  -12.93504  -0.29163  L
O-O2--0.801400       0    -6.4225   -13.16685  -1.18276  L
H-H-0.293600         0    -7.81422  -10.78473   2.67904  L
H-H-0.271900         0    -9.07953  -13.86953   2.8076   L
H-H1-0.088000        0    -8.07145  -12.97031   0.68461  L
H-HC--0.012200       0    -5.51189  -11.53971   1.50029  L
H-HC--0.012200       0    -6.5729   -10.91407   0.2384   L
H-H1-0.097600        0    -7.47141  -16.01459   3.79372  L
H-H1-0.097600        0    -9.02026  -15.48736   4.49075  L
H-H1-0.097600        0    -7.49948  -14.73257   5.02014  L
N-N--0.347900        0    -3.46237  -14.52799   1.91626  L
C-CT--0.263700       -1   -2.28462  -14.89648   2.72275  L
C-C-0.734100         0    -2.2478   -14.09198   4.04808  L
N-N--0.415700        0    -3.41716  -13.89578   4.68082  L
C-CT--0.149000       -1   -3.61485  -13.22652   5.97565  L
O-O--0.589400        0    -1.18519  -13.66146   4.49098  L
C-CT--0.000700       0    -1.01531  -14.71263   1.86421  L
C-CT-0.039000        0    -1.03815  -15.54298   0.55707  L
C-CT-0.048600        0    -0.73979  -14.71559  -0.70131  L
N-N2--0.529500       0    -1.68501  -13.59259  -0.8794   L
C-CA-0.807600        0    -1.38979  -12.36771  -1.26417  L
N-N2--0.862700       0    -0.20682  -12.02483  -1.66724  L
N-N2--0.862700       0    -2.30603  -11.45384  -1.24272  L
H-H-0.271900         0    -4.24389  -14.19219   4.17997  L
H-H-0.274700         0    -3.37907  -13.9473   1.08429  L
H-H-0.274700         0    -4.40292  -14.59635   2.29962  L
H-H1-0.156000        0    -2.35408  -15.94784   3.00302  L
H-HC-0.032700        0    -0.14562  -15.02045   2.44745  L
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H-HC-0.032700        0    -0.89307  -13.65121   1.64163  L
H-HC-0.028500        0    -2.00115  -16.03605   0.42283  L
H-HC-0.028500        0    -0.28771  -16.33077   0.63409  L
H-H1-0.068700        0    -0.79382  -15.36857  -1.57507  L
H-H1-0.068700        0     0.28326  -14.34229  -0.62639  L
H-H-0.345600         0    -2.67902  -13.72835  -0.72099  L
H-H-0.447800         0    -0.08564  -11.1205  -2.10456  L
H-H-0.447800         0     0.35792  -12.79191  -2.01408  L
H-H-0.447800         0    -2.09961  -10.55644  -1.66497  L
H-H-0.447800         0    -3.22749  -11.75676  -0.93477  L
H-H1-0.097600        0    -3.88606  -12.18221   5.81017  L
H-H1-0.097600        0    -2.694    -13.25727   6.56175  L
H-H1-0.097600        0    -4.41075  -13.72002   6.53457  L
N-N--0.415700        0    -0.27094  -8.98707   11.475   L
C-CT--0.149000      -1    -0.12224  -8.09312   10.32034  L
C-C-0.597300         0    -1.04457  -6.88137   10.49658  L
N-N--0.415700        0    -2.35893  -7.10846   10.44391  L
C-CT--0.149000       0    -3.37958  -6.12508   10.78828  L
O-O--0.567900        0    -0.56714  -5.78441   10.78622  L
C-CT--0.015200       0    -0.2887   -8.9053    9.02883  L
C-CA--0.001100       0     0.4518   -10.23864   9.02098  L
C-CA--0.190600       0     1.74775  -10.3512   9.57239  L
C-CA--0.190600       0    -0.17426  -11.38338   8.48795  L
C-CA--0.234100       0     2.39717  -11.59964   9.62243  L
C-CA--0.234100       0     0.48817  -12.62517   8.50148  L
C-C-0.322600         0     1.76876  -12.74059   9.07861  L
O-OH--0.557900       0     2.39494  -13.94423   9.09209  L
H-H-0.271900         0    -2.6372   -8.05882   10.25056  L
H-H-0.271900         0    -0.07665  -9.97557   11.3547  L
H-H-0.271900         0    -0.48148  -8.61582   12.39311  L
H-H1-0.087600        0     0.89696  -7.70609   10.33106  L
H-HC-0.029500        0     0.07094  -8.30468   8.19296  L
H-HC-0.029500        0    -1.34929  -9.10781   8.88365  L
H-HA-0.169900        0     2.25358  -9.48348   9.97367  L
H-HA-0.169900        0    -1.16965  -11.32647   8.06751  L
H-HA-0.165600        0     3.38306  -11.67773   10.05661  L
H-HA-0.165600        0     0.02277  -13.5074   8.08394  L
H-HO-0.399200        0     3.22382  -13.93343   9.57147  L
H-H1-0.097600        0    -3.34208  -5.29837   10.07998  L
H-H1-0.097600        0    -3.19557  -5.73399   11.79095  L
H-H1-0.097600        0    -4.36775  -6.58637   10.76229  L
N-N--0.415700        0     1.83256  -4.28907   11.90701  L
C-CT--0.059700      -1     2.23064  -3.05441   11.21304  L
C-C-0.597300         0     2.2556   -1.84169   12.15976  L
N-N--0.415700        0     1.23435  -1.68726   13.01045  L
C-CT--0.149000       0     1.11458  -0.59402   13.97537  L
O-O--0.567900        0     3.19703  -1.05121   12.10715  L
C-CT-0.130300        0     1.31801  -2.85293   9.96643  L
C-CT--0.043000       0     1.81112  -3.60456   8.7034   L
C-CT--0.320400       0     1.16844  -1.37489   9.55645  L
C-CT--0.066000       0     2.15619  -5.09059   8.84994  L
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H-H-0.271900          0      0.51075  -2.38965   12.983   L
H-H-0.271900          0      1.04896  -4.83286   11.54339  L
H-H-0.271900          0      2.344    -4.61146   12.71839  L
H-H1-0.086900         0      3.25437  -3.17245   10.86154  L
H-HC-0.018700         0      0.3171   -3.21662   10.20688  L
H-HC-0.023600         0      2.69347  -3.10562   8.31426  L
H-HC-0.023600         0      1.03964  -3.52596   7.93669  L
H-HC-0.088200         0      2.15058  -0.92639   9.4053   L
H-HC-0.088200         0      0.62628  -0.81801   10.32101  L
H-HC-0.088200         0      0.60237  -1.30129   8.62855  L
H-HC-0.018600         0      2.50693  -5.46624   7.89158  L
H-HC-0.018600         0      1.27309  -5.65481   9.13003  L
H-HC-0.018600         0      2.94632  -5.23761   9.58491  L
H-H1-0.097600         0      0.96542   0.35383   13.45533  L
H-H1-0.097600         0      2.0266   -0.51608   14.57184  L
H-H1-0.097600         0      0.27104  -0.76835   14.64514  L
N-N--0.415700         0      5.1011    1.00462   12.79682  L
C-CT--0.051800       -1      4.51794   2.35044   12.78033  L
C-C-0.597300          0      3.91688   2.69592   14.15074  L
N-N--0.415700         0      4.53456   3.63262   14.87972  L
C-CT--0.149000        0      4.08197   4.06958   16.20026  L
O-O--0.567900         0      2.89669   2.12702   14.52799  L
C-CT-0.110200         0      3.41179   2.44276   11.71377  L
C-CT-0.353100         0      3.89057   2.17777   10.2757  L
C-CT--0.412100        0      2.70405   2.23714   9.31641  L
C-CT--0.412100        0      4.94995   3.18143   9.80859  L
H-H-0.271900          0      5.37212   4.05505   14.51073  L
H-H-0.271900          0      4.4797    0.21073   12.63546  L
H-H-0.271900          0      5.99528   0.84069   13.24068  L
H-H1-0.092200         0      5.29573   3.07936   12.55551  L
H-HC-0.045700         0      2.96714   3.43824   11.75689  L
H-HC-0.045700         0      2.63125   1.71817   11.95252  L
H-HC--0.036100        0      4.30779   1.17721   10.21609  L
H-HC-0.100000         0      2.25313   3.22909   9.33266  L
H-HC-0.100000         0      1.95727   1.50285   9.61566  L
H-HC-0.100000         0      3.03951   2.00239   8.30555  L
H-HC-0.100000         0      5.19907   2.99201   8.76772  L
H-HC-0.100000         0      5.86266   3.06919   10.39213  L
H-HC-0.100000         0      4.57705   4.20177   9.90533  L
H-H1-0.097600         0      4.74621   4.84072   16.59457  L
H-H1-0.097600         0      4.07264   3.22205   16.88919  L
H-H1-0.097600         0      3.06887   4.47164   16.13304  L
N-N--0.415700         0    -12.40978   0.40531   9.36113  L
C-CT--0.001400       -1    -11.27335  -0.00219   10.19624  L
C-C-0.597300          0    -10.43664  -1.10306   9.53902  L
O-O--0.567900         0    -9.23409  -0.94438   9.31826  L
C-CT--0.015200        0    -11.76896  -0.40154   11.59437  L
C-CA--0.001100        0    -12.49771   0.7169    12.31601  L
C-CA--0.190600        0    -11.76915   1.80962   12.82561  L
C-CA--0.190600        0    -13.90066   0.68205   12.45229  L
C-CA--0.234100        0    -12.44115   2.86638   13.46872  L
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C-CA--0.234100       0    -14.57501   1.73708   13.09853  L
C-C-0.322600         0    -13.84368   2.83274   13.60782  L
O-OH--0.557900       0    -14.48067   3.85879   14.22837  L
H-H-0.271900         0    -13.16293   0.9316    9.78724   L
H-H-0.271900         0    -12.38429   0.28373   8.35363   L
H-H1-0.087600        0    -10.61464   0.86001   10.31126  L
H-HC-0.029500        0    -10.90968  -0.69748   12.19826  L
H-HC-0.029500        0    -12.42811  -1.26725   11.51362  L
H-HA-0.169900        0    -10.69243   1.84195   12.72806  L
H-HA-0.169900        0    -14.46717  -0.15486   12.06694  L
H-HA-0.165600        0    -11.8994    3.70999   13.86996  L
H-HA-0.165600        0    -15.649     1.70923   13.20603  L
H-HO-0.399200        0    -15.41437   3.68479   14.35589  L
N-N--0.347900        0    -11.10814  -2.21197   9.22706   L
C-CT--0.263700      -1    -10.5904   -3.40658   8.56168   L
C-C-0.734100         0    -11.69021  -3.94556   7.64416   L
O-O--0.589400        0    -12.85178  -3.96693   8.0507    L
C-CT--0.000700       0    -10.08127  -4.38702   9.64138   L
C-CT-0.039000        0    -11.16545  -5.05378   10.51168  L
C-CT-0.048600        0    -11.61266  -6.39758   9.92737   L
N-N2--0.529500       0    -12.72977  -6.99793   10.67651  L
C-CA-0.807600        0    -13.15075  -8.24412   10.55381  L
N-N2--0.862700       0    -12.59448  -9.10325   9.75068   L
N-N2--0.862700       0    -14.16531  -8.66333   11.25716  L
H-H-0.274700         0    -12.10524  -2.20432   9.39919   L
H-H1-0.156000        0    -9.74841   -3.11868   7.94344   L
H-HC-0.032700        0    -9.42102   -3.82762   10.30639  L
H-HC-0.032700        0    -9.45752   -5.15105   9.1811    L
H-HC-0.028500        0    -12.02199  -4.3888    10.6254   L
H-HC-0.028500        0    -10.74734  -5.24124   11.50145  L
H-H1-0.068700        0    -10.7541   -7.07015   9.95043   L
H-H1-0.068700        0    -11.91912  -6.26527   8.89045   L
H-H-0.345600         0    -13.24905  -6.38992   11.28239  L
H-H-0.447800         0    -12.89332  -10.04946   9.65745  L
H-H-0.447800         0    -11.81508  -8.78589   9.1548    L
H-H-0.447800         0    -14.47196  -9.6115    11.15417  L
H-H-0.447800         0    -14.63517  -8.04143   11.88811  L
N-N--0.415700        0    -11.34674  -4.26319   6.40189   L
C-CT--0.003100      -1    -12.28928  -4.52956   5.30842   L
C-C-0.597300         0    -13.15903  -5.79911   5.45711   L
N-N--0.415700        0    -12.78026  -6.76078   6.30751   L
C-CT--0.149000      -1    -13.549    -7.97245   6.59726   L
O-O--0.567900        0    -14.19027  -5.89877   4.788     L
C-CT--0.003600       0    -11.53301  -4.5451    3.96886   L
C-CT--0.064500       0    -11.03167  -3.13571   3.62352   L
C-C-0.695100         0    -10.38203  -3.03237   2.24963   L
O-O--0.608600        0    -9.6502    -3.90351   1.7917    L
N-N--0.940700        0    -10.5896   -1.93033   1.56898   L
H-H-0.271900         0    -10.35709  -4.30241   6.21817   L
H-H-0.271900         0    -11.85307  -6.66083   6.71768   L
H-H1-0.085000        0    -12.99991  -3.70155   5.27548   L
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H-HC-0.017100        0    -12.20863  -4.87299   3.17739  L
H-HC-0.017100        0    -10.69374  -5.24002   4.02557  L
H-HC-0.035200        0    -10.29954  -2.815     4.36398  L
H-HC-0.035200        0    -11.8767   -2.44697   3.66233  L
H-H-0.425100         0    -9.81808   -1.69721   0.95238  L
H-H-0.425100         0    -11.18099  -1.21104   1.95955  L
H-H1-0.097600        0    -12.8607   -8.7812    6.84583  L
H-H1-0.097600        0    -14.13006  -8.26417   5.7213   L
H-H1-0.097600        0    -14.22322  -7.78772   7.43314  L
N-N--0.347900        0    -14.9044   -14.74251  -4.34608  L
C-CT--0.240000       -1   -14.8533   -13.2727   -4.39715  L
C-C-0.734100         0    -15.59522  -12.72543  -5.64496  L
N-N-0.415700         0    -16.01727  -11.4587   -5.7346   L
C-CT-0.149000        0    -15.99155  -10.40703  -4.72744  L
O-O--0.589400        0    -15.78377  -13.47316  -6.59293  L
C-CT--0.009400       0    -13.36301  -12.82352  -4.43307  L
C-CT-0.018700        0    -12.50253  -13.14951  -3.1879   L
C-CT--0.047900       0    -11.1106   -12.47029  -3.23913  L
C-CT--0.014300       0    -10.15388  -12.99099  -2.14622  L
N-N3--0.385400       0    -8.85292   -12.26789  -2.11838  L
H-H-0.274700         0    -16.43667  -11.26726  -6.63191  L
H-H-0.271900         0    -14.66661  -15.25676  -3.50366  L
H-H-0.271900         0    -15.12251  -15.26628  -5.19232  L
H-H1-0.142600        0    -15.32181  -12.8914   -3.4879   L
H-HC-0.036200        0    -13.33281  -11.74723  -4.57962  L
H-HC-0.036200        0    -12.88282  -13.27428  -5.30481  L
H-HC-0.010300        0    -12.36964  -14.23052  -3.1261   L
H-HC-0.010300        0    -13.02367  -12.81147  -2.29103  L
H-HC-0.062100        0    -11.23737  -11.39258  -3.1188   L
H-HC-0.062100        0    -10.65614  -12.65893  -4.21358  L
H-HP-0.113500        0    -9.9697    -14.05451  -2.32174  L
H-HP-0.113500        0    -10.63547  -12.8896   -1.16863  L
H-H-0.340000         0    -8.41312   -12.16978  -3.02315  L
H-H-0.340000         0    -8.14343   -12.74593  -1.55745  L
H-H-0.340000         0    -8.92567   -11.32668  -1.72563  L
H-H1-0.097600        0    -15.64697  -10.78135  -3.76443  L
H-H1-0.097600        0    -16.99503  -9.99834   -4.59783  L
H-H1-0.097600        0    -15.33129  -9.60327   -5.05404  L
N-N--0.254800        0    -15.83492  -8.98801   -1.6157   L
C-CT--0.026600       -1   -14.74854  -8.04063   -1.82991  L
C-C-0.589600         0    -13.64467  -8.55461   -2.75857  L
O-O--0.574800        0    -13.49191  -9.75321   -3.00479  L
C-CT--0.007000       0    -14.21884  -7.72805   -0.42383  L
C-CT-0.018900        0    -15.47757  -7.83466    0.43805  L
C-CT-0.019200        0    -16.20703  -9.01496   -0.20996  L
H-H1-0.064100        0    -15.1755   -7.13065   -2.2542   L
H-HC-0.025300        0    -13.77551  -6.73446   -0.36441  L
H-HC-0.025300        0    -13.49841  -8.48834   -0.11468  L
H-HC-0.021300        0    -16.07541  -6.92838    0.32697  L
H-HC-0.215300        0    -15.24742  -8.00962    1.4933   L
H-H1-0.039100        0    -15.86708  -9.9513     0.23501  L
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H-H1-0.039100        0    -17.28615  -8.91184  -0.08747  L
N-N--0.415700        0    -12.91106  -7.61241  -3.33798  L
C-CT--0.038900       -1   -11.70454  -7.72655  -4.18017  L
C-C-0.597300         0    -11.12107  -6.31853  -4.16149  L
O-O--0.567900        0    -11.8855  -5.35922  -4.28194  L
C-CT-0.365400        0    -12.05488  -8.15269  -5.61952  L
O-OH--0.676100       0    -12.8477  -9.32569  -5.58253  L
C-CT--0.243800       0    -10.8104  -8.48324  -6.43669  L
H-H-0.271900         0    -13.1517  -6.654    -3.11541  L
H-H1-0.100700        0    -10.99341  -8.42794  -3.73925  L
H-H1-0.004300        0    -12.61719  -7.35996  -6.1148   L
H-HC-0.064200        0    -10.17083  -7.60483  -6.52186  L
H-HC-0.064200        0    -11.10496  -8.80025  -7.43741  L
H-HC-0.064200        0    -10.25259  -9.28737  -5.95622  L
H-HO-0.410200        0    -12.79214  -9.61957  -4.65818  L
N-N--0.415700        0    -9.82408  -6.17429  -3.92275  L
C-CT--0.001400       -1   -9.15113  -4.90767  -3.61629  L
C-C-0.597300         0    -9.55987  -3.75076  -4.53887  L
O-O--0.567900        0    -10.05875  -2.75329  -4.03207  L
C-CT--0.015200       0    -7.66047  -5.18951  -3.61957  L
C-CA--0.001100       0    -6.80356  -3.95276  -3.75518  L
C-CA--0.190600       0    -6.17896  -3.6863   -4.98724  L
C-CA--0.190600       0    -6.72962  -3.01947  -2.70368  L
C-CA--0.234100       0    -5.56239  -2.44533  -5.19942  L
C-CA--0.234100       0    -6.1094   -1.77541  -2.91669  L
C-C-0.322600         0    -5.57624  -1.4683   -4.18507  L
O-OH--0.557900       0    -5.12873  -0.21974  -4.46502  L
H-H-0.271900         0    -9.25896  -7.02179  -3.85108  L
H-H1-0.087600        0    -9.41818  -4.60577  -2.60255  L
H-HC-0.029500        0    -7.41362  -5.87826  -4.42952  L
H-HC-0.029500        0    -7.47666  -5.68972  -2.67535  L
H-HA-0.169900        0    -6.22144  -4.39594  -5.80377  L
H-HA-0.169900        0    -7.19539  -3.22056  -1.7451   L
H-HA-0.165600        0    -5.12275  -2.21389  -6.1581   L
H-HA-0.165600        0    -6.10497  -1.03974  -2.12413  L
H-HO-0.399200        0    -4.9255    0.28448  -3.65082  L
N-N--0.415700        0    -9.46796  -3.91482  -5.86721  L
C-CT-0.014300        -1   -9.87895  -2.93428  -6.89483  L
C-C-0.597300         0    -11.345   -2.45867  -6.85476  L
O-O--0.567900        0    -11.72635  -1.60594  -7.64641  L
C-CT--0.204100       0    -9.45994  -3.4515   -8.28566  L
C-C-0.713000         0    -8.14717  -2.83397  -8.73147  L
O-O--0.593100        0    -7.16584  -2.785    -8.01078  L
N-N--0.919100        0    -8.09191  -2.28409  -9.91372  L
H-H-0.271900         0    -9.00122  -4.75236  -6.17546  L
H-H1-0.104800        0    -9.31033  -2.02379  -6.69603  L
H-HC-0.079700        0    -10.22501  -3.19002  -9.01835  L
H-HC-0.079700        0    -9.35742  -4.53533  -8.2861   L
H-H-0.419600         0    -7.24027  -1.8087   -10.14007  L
H-H-0.419600         0    -8.96793  -2.09566  -10.39531  L
N-N--0.415700        0    -12.14048  -2.95592  -5.91092  L
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C-CT--0.002400       -1   -13.44874  -2.43265  -5.53996  L
C-C-0.597300         0    -13.53257  -2.05397  -4.06009  L
O-O--0.567900        0    -13.99782  -0.96947  -3.72435  L
C-CT--0.034300       0    -14.52332  -3.45988  -5.92165  L
C-CA-0.011800        0    -15.93315  -3.02341  -5.57214  L
C-CA--0.125600       0    -16.62582  -2.14233  -6.4234   L
C-CA--0.125600       0    -16.54163  -3.46686  -4.38096  L
C-CA--0.170400       0    -17.92243  -1.71295  -6.08977  L
C-CA--0.170400       0    -17.83911  -3.03752  -4.04862  L
C-CA--0.107200       0    -18.52937  -2.16076  -4.90372  L
H-H-0.271900         0    -11.71984  -3.64177  -5.30054  L
H-H1-0.097800        0    -13.64837  -1.51915  -6.10489  L
H-HC-0.029500        0    -14.31078  -4.40625  -5.42267  L
H-HC-0.029500        0    -14.47136  -3.63637  -6.99729  L
H-HA-0.133000        0    -16.16068  -1.78015  -7.33019  L
H-HA-0.133000        0    -16.00967  -4.12041  -3.70748  L
H-HA-0.143000        0    -18.44903  -1.02757  -6.74036  L
H-HA-0.143000        0    -18.30542  -3.36183  -3.12918  L
H-HA-0.129700        0    -19.52222  -1.81785  -4.64534  L
N-N--0.415700        0    -13.06961  -2.93658  -3.17175  L
C-CT-0.033700        -1   -13.02404  -2.70098  -1.73116  L
C-C-0.597300         0    -12.35326  -1.36344  -1.37379  L
O-O--0.567900        0    -12.93112  -0.55547  -0.64973  L
C-CT--0.182500       0    -12.33115  -3.89433  -1.06024  L
H-H-0.271900         0    -12.64642  -3.77846  -3.53699  L
H-H1-0.082300        0    -14.04906  -2.64638  -1.36053  L
H-HC-0.060300        0    -12.83363  -4.81904  -1.33629  L
H-HC-0.060300        0    -12.37331  -3.77435   0.02353  L
H-HC-0.060300        0    -11.28547  -3.94383  -1.36498  L
N-N--0.415700        0    -11.16469  -1.11577  -1.93413  L
C-CT--0.087500       -1   -10.43214   0.14875  -1.80555  L
C-C-0.597300         0    -11.25046   1.35389  -2.24971  L
O-O--0.567900        0    -11.17228   2.398    -1.62292  L
C-CT-0.298500        0    -9.07286   0.073    -2.53295  L
C-CT--0.319200       0    -9.14155   0.28258  -4.05112  L
C-CT--0.319200       0    -8.06818   1.0797   -1.96934  L
H-H-0.271900         0    -10.77415  -1.82172  -2.54875  L
H-H1-0.096900        0    -10.22445   0.29154  -0.74443  L
H-HC--0.029700       0    -8.66608  -0.92094  -2.35387  L
H-HC-0.079100        0    -8.19455  -0.02686  -4.48771  L
H-HC-0.079100        0    -9.31611   1.33396  -4.2854   L
H-HC-0.079100        0    -9.93716  -0.31571  -4.48675  L
H-HC-0.079100        0    -7.82333   0.80898  -0.94447  L
H-HC-0.079100        0    -8.48729   2.08519  -1.99661  L
H-HC-0.079100        0    -7.1519    1.06249  -2.557    L
N-N--0.415700        0    -12.03804   1.21482  -3.31724  L
C-CT--0.087500       -1   -12.83035   2.29673  -3.90848  L
C-C-0.597300         0    -13.95847   2.73953  -2.98615  L
O-O--0.567900        0    -14.11684   3.93064  -2.7323   L
C-CT-0.298500        0    -13.3711   1.92519  -5.30682  L
C-CT--0.319200       0    -13.98811   3.14322  -6.00454  L
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C-CT--0.319200       0    -12.25721   1.38868  -6.21637  L
H-H-0.271900         0    -12.11264   0.29403  -3.71979  L
H-H1-0.096900        0    -12.17308   3.1589   -4.02993  L
H-HC--0.029700       0    -14.13837   1.15769  -5.21402  L
H-HC-0.079100        0    -14.33388   2.86441  -7.00095  L
H-HC-0.079100        0    -13.24658   3.93712  -6.10106  L
H-HC-0.079100        0    -14.84105   3.51577  -5.43761  L
H-HC-0.079100        0    -11.86249   0.45319  -5.82723  L
H-HC-0.079100        0    -11.45552   2.12275  -6.28902  L
H-HC-0.079100        0    -12.65628   1.19542  -7.21301  L
N-N--0.415700        0    -14.73102   1.78225  -2.46805  L
C-CT--0.087500       -1   -15.7625    2.03809  -1.45199  L
C-C-0.597300         0    -15.16016   2.7324   -0.23647  L
O-O--0.567900        0    -15.62418   3.79047   0.17728  L
C-CT-0.298500        0    -16.49324   0.73613  -1.06072  L
C-CT--0.319200       0    -17.56947   0.98016   0.00581  L
C-CT--0.319200       0    -17.18893   0.10273  -2.27462  L
H-H-0.271900         0    -14.51988   0.82829  -2.7394   L
H-H1-0.096900        0    -16.49588   2.72467  -1.87492  L
H-HC--0.029700       0    -15.77185   0.01938  -0.66665  L
H-HC-0.079100        0    -18.0955    0.05087   0.22363  L
H-HC-0.079100        0    -18.28405   1.72484  -0.34652  L
H-HC-0.079100        0    -17.1118    1.3335    0.93013  L
H-HC-0.079100        0    -17.90112   0.80597  -2.70715  L
H-HC-0.079100        0    -17.71643  -0.8003   -1.97003  L
H-HC-0.079100        0    -16.45752  -0.17198  -3.03385  L
N-N--0.516300        0    -14.13137   2.12324   0.33836  L
C-CT-0.038100        -1   -13.51753   2.51985   1.60158  L
C-C-0.536600         0    -12.68012   3.80553   1.5039   L
O-O--0.581900        0    -12.5786    4.54933   2.47207  L
C-CT--0.030300       0    -12.72692   1.29085   2.07771  L
C-C-0.799400         0    -12.56891   1.21492   3.59035  L
O-O2--0.801400       0    -12.19794   2.24158   4.19455  L
O-O2--0.801400       0    -12.70458   0.09599   4.13185  L
H-H-0.293600         0    -13.79      1.27002  -0.09119  L
H-H1-0.088000        0    -14.31331   2.7087    2.32366  L
H-HC--0.012200       0    -11.75064   1.26959   1.5928   L
H-HC--0.012200       0    -13.26036   0.38726   1.77539  L
N-N--0.516300        0    -12.11498   4.14049   0.34294  L
C-CT-0.038100        -1   -11.46891   5.44111   0.13384  L
C-C-0.536600         0    -12.43617   6.62533   0.00781  L
O-O--0.581900        0    -11.99815   7.76997   0.12326  L
C-CT--0.030300       0    -10.40997   5.39919  -0.99063  L
C-C-0.799400         0    -9.08995    4.73476  -0.55496  L
O-O2--0.801400       0    -8.91731    4.40562   0.64167  L
O-O2--0.801400       0    -8.14959    4.61481  -1.37514  L
H-H-0.293600         0    -12.14595   3.4848   -0.43178  L
H-H1-0.088000        0    -10.91927   5.67398   1.04598  L
H-HC--0.012200       0    -10.16757   6.42352  -1.27797  L
H-HC--0.012200       0    -10.8178    4.90613  -1.87284  L
N-N--0.415700        0    -13.74438   6.38307  -0.11002  L
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C-CT--0.058100       -1   -14.77566   7.42668  -0.10401  L
C-C-0.597300         0    -15.74361   7.24509   1.0711   L
N-N--0.415700        0    -16.65883   6.27633   1.00102  L
C-CT--0.149000       0    -17.63962   5.96436   2.03727  L
O-O--0.567900        0    -15.63112   7.9619    2.06846  L
C-CT--0.007400       0    -15.44743   7.50542  -1.48066  L
C-CC-0.186800        0    -14.4959   8.02749  -2.52795  L
N-NB--0.543200       0    -14.06234   9.35     -2.62634  L
C-CW--0.220700       0    -13.85767   7.27642  -3.47019  L
C-CR-0.163500        0    -13.17731   9.36797  -3.63356  L
N-NA--0.279500       0    -13.03326   8.13825  -4.16076  L
H-H-0.271900         0    -14.02089   5.41099  -0.19366  L
H-H-0.271900         0    -16.55002   5.61733   0.23712  L
H-H1-0.136000        0    -14.3063   8.39751   0.05758  L
H-HC-0.036700        0    -16.29713   8.1866   -1.42575  L
H-HC-0.036700        0    -15.81059   6.51957  -1.77563  L
H-H4-0.186200        0    -13.96693   6.21027  -3.61165  L
H-H-0.333900         0    -12.41451   7.89348  -4.92179  L
H-H5-0.143500        0    -12.65152   10.25197  -3.96863  L
H-H1-0.097600        0    -18.10709   6.88219   2.39876  L
H-H1-0.097600        0    -17.14635   5.45857   2.86861  L
H-H1-0.097600        0    -18.40892   5.30709   1.62917  L
N-N--0.415700        0    -13.95211   6.38132   3.9706   L
C-CT--0.023700       -1   -13.13098   7.06228   4.97188  L
C-C-0.597300         0    -12.9473   8.58147   4.72329  L
N-N--0.415700        0    -13.65085   9.16871   3.74952  L
C-CT--0.149000       0    -13.74767   10.60747   3.51791  L
O-O--0.567800        0    -12.21124   9.25165   5.46124  L
C-CT-0.034200        0    -11.77988   6.35293   5.16462  L
C-CT-0.001800        0    -11.93975   5.04645   5.94157  L
S-S--0.273700        0    -10.36838   4.34601   6.51322  L
C-CT--0.053600       0    -11.00036   2.87364   7.35811  L
H-H-0.271900         0    -14.23852   8.57543   3.16883  L
H-H-0.271900         0    -13.5607   5.5534    3.52057  L
H-H-0.271900         0    -14.77156   6.8149    3.55593  L
H-H1-0.088000        0    -13.66653   6.99492   5.91861  L
H-HC-0.024100        0    -11.12482   6.99115   5.75548  L
H-HC-0.024100        0    -11.30354   6.1644    4.20149  L
H-H1-0.044000        0    -12.45665   4.32614   5.31176  L
H-H1-0.044000        0    -12.5599   5.23091   6.81859  L
H-H1-0.068400        0    -11.64612   3.17513   8.18212  L
H-H1-0.068400        0    -10.16573   2.28916   7.74463  L
H-H1-0.068400        0    -11.57361   2.26763   6.65531  L
H-H1-0.097600        0    -12.75465   11.05519   3.50387  L
H-H1-0.097600        0    -14.3472   11.06807   4.30478  L
H-H1-0.097600        0    -14.2361   10.78506   2.55711  L
N-N--0.415700        0    -11.66734   10.38468   1.0771   L
C-CT--0.059700       -1   -10.30138   10.80379   1.39976  L
C-C-0.597300         0    -9.94451   12.00196   0.49685  L
N-N--0.415700        0    -10.05928   13.2173   1.04571  L
C-CT--0.149000       0    -9.78944   14.48604   0.36807  L
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O-O--0.567900        0    -9.59676   11.84437  -0.67262  L
C-CT-0.130300        0    -9.34278   9.59962   1.21044  L
C-CT--0.043000       0    -9.58416   8.48949   2.26395  L
C-CT--0.320400       0    -7.85273   9.9848    1.18779  L
C-CT--0.066000       0    -9.29468   8.86823   3.72413  L
H-H-0.271900         0    -10.37591   13.2498   1.99838  L
H-H-0.271900         0    -11.81404   9.38039   0.9583   L
H-H-0.271900         0    -12.19473   10.96009   0.43164  L
H-H1-0.086900        0    -10.25547   11.13588   2.43365  L
H-HC-0.018700        0    -9.5588    9.16498   0.23203  L
H-HC-0.023600        0    -8.97156   7.62564   2.00369  L
H-HC-0.023600        0    -10.62136   8.16267   2.21402  L
H-HC-0.088200        0    -7.2654    9.11587   0.90546  L
H-HC-0.088200        0    -7.52522   10.3681   2.15085  L
H-HC-0.088200        0    -7.65538   10.73952   0.43344  L
H-HC-0.018600        0    -9.9292    9.69365   4.04152  L
H-HC-0.018600        0    -8.25067   9.14009   3.85682  L
H-HC-0.018600        0    -9.5023    8.00684   4.35388  L
H-H1-0.097600        0    -10.50582   15.2433   0.69015  L
H-H1-0.097600        0    -9.87939   14.36611  -0.71455  L
H-H1-0.097600        0    -8.77907   14.82605   0.60206  L
N-N--0.415703        0    -7.00699   13.10291  -0.90173  L
C-CT--0.058100       -1   -5.62441   12.77608  -1.24431  L
C-C-0.597300         0    -5.38191   11.26424  -1.19787  L
O-O--0.567900        0    -4.89208   10.7009  -0.21343  L
C-CT--0.007400       0    -4.69559   13.54723  -0.28694  L
C-CC-0.186800        0    -4.95966   15.03269  -0.22055  L
N-NB--0.543200       0    -5.94109   15.64957   0.5647   L
C-CW--0.220700       0    -4.28615   15.98492  -0.92587  L
C-CR-0.163500        0    -5.83478   16.96289   0.30704  L
N-NA--0.279500       0    -4.8506    17.19395  -0.58058  L
H-H-0.271900         0    -7.12861   13.80365  -0.17686  L
H-H-0.271900         0    -7.78804   12.48412  -1.11371  L
H-H1-0.136000        0    -5.41739   13.12481  -2.25624  L
H-HC-0.036700        0    -3.65896   13.38287  -0.57959  L
H-HC-0.036700        0    -4.81905   13.15661   0.71746  L
H-H4-0.186200        0    -3.47041   15.81076  -1.6141   L
H-H-0.333900         0    -4.57914   18.10524  -0.92733  L
H-H5-0.143500        0    -6.45495   17.7318   0.74995  L
N-N--0.415700        0    -5.75345   10.58986  -2.28677  L
C-CT--0.087500       -1   -5.70707   9.12538  -2.40796  L
C-C-0.597300         0    -4.28724   8.66885  -2.75447  L
O-O--0.567900        0    -3.97418   8.25189  -3.86788  L
C-CT-0.298500        0    -6.77769   8.62108  -3.40544  L
C-CT--0.319200       0    -6.98232   7.11347  -3.24872  L
C-CT--0.319200       0    -8.15097   9.2713   -3.16566  L
H-H-0.271900         0    -6.1941    11.10834  -3.03197  L
H-H1-0.096900        0    -5.9658    8.70491  -1.4422   L
H-HC--0.029700       0    -6.4709    8.84993  -4.42445  L
H-HC-0.079100        0    -6.0518    6.575    -3.42281  L
H-HC-0.079100        0    -7.72447   6.76515  -3.96747  L
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 H-HC-0.079100        0    -7.35696   6.89661  -2.25093  L
 H-HC-0.079100        0    -8.46859   9.12269  -2.13283  L
 H-HC-0.079100        0    -8.8905    8.8184   -3.82821  L
 H-HC-0.079100        0    -8.1224    10.33705  -3.38632  L
 N-N--0.415700        0    -3.38716   8.85058  -1.79402  L
 C-CT--0.002400       -1   -1.9486    8.71943  -1.98873  L
 C-C-0.597300         0    -1.46362   7.30081  -1.66658  L
 O-O--0.567900        0    -1.9659    6.64705  -0.74577  L
 C-CT--0.034300       0    -1.21652   9.75978  -1.12769  L
 C-CA-0.011800        0    -1.29237   11.22301  -1.5519   L
 C-CA--0.125600       0    -2.1334    11.68257  -2.59088  L
 C-CA--0.125600       0    -0.44638   12.14209  -0.90265  L
 C-CA--0.170400       0    -2.11768   13.03545  -2.97574  L
 C-CA--0.170400       0    -0.43615   13.49591  -1.28061  L
 C-CA--0.107200       0    -1.26618   13.94205  -2.32236  L
 H-H-0.271900         0    -3.71688   9.27057  -0.93407  L
 H-H1-0.097800        0    -1.70182   8.91644  -3.03298  L
 H-HC-0.029500        0    -0.15837   9.49295  -1.1198   L
 H-HC-0.029500        0    -1.57656   9.67929  -0.10161  L
 H-HA-0.133000        0    -2.7693    11.01024  -3.14105  L
 H-HA-0.133000        0     0.22067   11.80205  -0.12079  L
 H-HA-0.143000        0    -2.72875   13.37336  -3.80177  L
 H-HA-0.143000        0     0.235     14.18645  -0.78794  L
 H-HA-0.129700        0    -1.22645   14.97597  -2.63615  L
 N-N--0.347900        0    -0.48526   6.82539  -2.44304  L
 C-CT--0.263700       -1    0.13896   5.49636  -2.36466  L
 C-C-0.734100         0     1.39192   5.39457  -3.23415  L
 O-O--0.589400        0     1.88779   6.41835  -3.6914   L
 C-CT--0.000700       0    -0.89793   4.42666  -2.76718  L
 C-CT-0.039000        0    -1.49791   4.5913   -4.17089  L    H-H1
1046  0.        0.
 C-CT-0.048600        0    -2.62964   3.57976  -4.32507  H
 N-N2--0.529500       0    -3.28619   3.73538  -5.61587  H
 C-CA-0.807600        0    -4.53541   3.33051  -5.81629  H
 N-N2--0.862700       0    -5.24168   2.80291  -4.82451  H
 N-N2--0.862700       0    -5.08488   3.44058  -7.04089  H
 H-H-0.274700         0    -0.18063   7.40965  -3.21969  L
 H-H1-0.156000        0     0.44931   5.30314  -1.33787  L
 H-HC-0.032700        0    -1.70416   4.45504  -2.0436   L
 H-HC-0.032700        0    -0.45669   3.43347  -2.6964   L
 H-HC-0.028500        0    -0.73395   4.41508  -4.92873  L
 H-HC-0.028500        0    -1.90558   5.59536  -4.29483  L
 H-H1-0.068700        0    -3.36489   3.76515  -3.53806  H
 H-H1-0.068700        0    -2.24396   2.56541  -4.18991  H
 H-H-0.345600         0    -2.73539   3.9015   -6.44559  H
 H-H-0.447800         0    -6.19663   2.53842  -5.07827  H
 H-H-0.447800         0    -4.82348   2.33975  -4.0025   H
 H-H-0.447800         0    -6.05871   3.14816  -7.10316  H
 H-H-0.447800         0    -4.78655   4.14442  -7.70624  H
 N-N--0.415700        0     1.89438   4.18256  -3.47032  L
 C-CT--0.025200       -1    3.03929   3.90702  -4.33563  L
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 C-C-0.597300          0     2.69698   3.74726  -5.81676  L
 O-O--0.567900         0     1.55882   3.50559  -6.22527  L
 H-H-0.271900          0     1.4278    3.37615  -3.06938  L
 H-H1-0.069800         0     3.50215   2.97677  -4.0071   L
 H-H1-0.069800         0     3.76956   4.70504  -4.21843  L
 N-N--0.516300         0     3.74505   3.86152  -6.62194  L
 C-CT-0.039700         0     3.8253    3.59434  -8.06023  L
 C-C-0.536600          0     3.30528   2.19778  -8.44073  L
 O-O--0.581900         0     2.68061   2.03445  -9.4884   L
 C-CT-0.056000         0     5.29033   3.82006  -8.44208  L
 C-CT-0.013600         0     5.66131   3.60379  -9.90919  L
 C-C-0.805400          0     7.09286   4.10479  -10.14634  L
 O-O2--0.818800        0     8.02963   3.63728  -9.45759  L
 O-O2--0.818800        0     7.2974    5.00888  -10.98303  L
 H-H-0.293600          0     4.6049    4.16701  -6.17494  L
 H-H1-0.110500         0     3.225     4.32526  -8.60029  L
 H-HC--0.017300        0     5.92044   3.17952  -7.82246  L
 H-HC--0.017300        0     5.513     4.85809  -8.20019  L
 H-HC--0.042500        0     4.95929   4.15359  -10.54056  L
 H-HC--0.042500        0     5.59417   2.54087  -10.15077  L
 N-N--0.516300         0     3.47483   1.2025   -7.56202  L
 C-CT-0.038100        -1     2.9366   -0.1566   -7.71175  L
 C-C-0.536600          0     1.39913  -0.23265  -7.85165  L
 O-O--0.581900         0     0.88157  -1.27053  -8.27341  L
 C-CT--0.030300        0     3.48538  -1.07284  -6.60419  L
 C-C-0.799400          0     2.8871   -0.89064  -5.20967  L
 O-O2--0.801400        0     2.65012   0.25585  -4.77163  L
 O-O2--0.801400        0     2.73911  -1.93355  -4.52618  L
 H-H-0.293600          0     3.90354   1.43342  -6.67656  L
 H-H1-0.088000         0     3.33345  -0.54133  -8.65169  L
 H-HC--0.012200        0     4.56033  -0.94137  -6.52257  L
 H-HC--0.012200        0     3.32744  -2.10369  -6.91586  L
 N-N--0.415700         0     0.68009   0.86603  -7.58061  L
 C-CT--0.058100        0    -0.76532   1.03156  -7.7926   L    H-HC
1102  0.        0.
 C-C-0.597300          0    -1.14091   2.23568  -8.6886   L
 O-O--0.567900         0    -2.31744   2.60111  -8.77431  L
 C-CT--0.007400        0    -1.44833   1.09129  -6.41945  H
 C-CC-0.186800         0    -1.47453  -0.20486  -5.67207  H
 N-NB--0.543200        0    -2.46797  -1.12569  -5.92065  H
 C-CW--0.220700        0    -0.61369  -0.68599  -4.72082  H
 C-CR-0.163500         0    -2.21214  -2.13323  -5.11714  H
 N-NA--0.279500        0    -1.09123  -1.92557  -4.38234  H
 H-H-0.271900          0     1.19995   1.63764  -7.17264  L
 H-H1-0.136000         0    -1.14918   0.14771  -8.30359  L
 H-HC-0.036700         0    -2.4934    1.38215  -6.56854  H
 H-HC-0.036700         0    -0.9482    1.87005  -5.83283  H
 H-H4-0.186200         0     0.27792  -0.27813  -4.27447  H
 H-H-0.333900          0    -0.70284  -2.54015  -3.67075  H
 H-H5-0.143500         0    -2.79664  -3.03646  -5.02256  H
 N-N--0.415700         0    -0.1928    2.81756  -9.43666  L
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C-CT--0.051800       -1   -0.4756    3.71144  -10.5784  L
C-C-0.597300         0    -1.34996   2.97811  -11.60204  L
O-O--0.567900        0    -2.47816   3.37751  -11.87855  L
C-CT--0.110200       0     0.86024   4.19515  -11.18181  L
C-CT-0.353100        0     0.73316   5.04783  -12.45909  L
C-CT--0.412100       0    -0.06322   6.33275  -12.24116  L
C-CT--0.412100       0     2.12744   5.42794  -12.95458  L
H-H-0.271900         0     0.76202   2.48704  -9.31462  L
H-H1-0.092200        0    -1.03563   4.57686  -10.2296  L
H-HC-0.045700        0     1.4709    3.32487  -11.42455  L
H-HC-0.045700        0     1.39843   4.77053  -10.43    L
H-HC--0.036100       0     0.24397   4.46101  -13.23665  L
H-HC-0.100000        0    -1.08197   6.10545  -11.93175  L
H-HC-0.100000        0    -0.10414   6.90165  -13.16989  L
H-HC-0.100000        0     0.41936   6.94317  -11.47775  L
H-HC-0.100000        0     2.64219   6.03084  -12.20487  L
H-HC-0.100000        0     2.04983   6.00059  -13.87889  L
H-HC-0.100000        0     2.71327   4.52923  -13.14825  L
N-N--0.415700        0    -0.84476   1.84524  -12.08583  L
C-CT--0.024900       -1   -1.49957   0.87161  -12.96735  L
C-C-0.597300         0    -2.96593   0.57053  -12.60847  L
O-O--0.567900        0    -3.81195   0.52044  -13.50325  L
C-CT-0.211700        0    -0.67764  -0.42431  -12.92845  L
O-OH--0.654600       0    -0.56367  -0.85996  -11.58383  L
H-H-0.271900         0     0.06101   1.59054  -11.71546  L
H-H1-0.084300        0    -1.4825    1.26121  -13.98505  L
H-H1-0.035200        0     0.31807  -0.23067  -13.33117  L
H-H1-0.035200        0    -1.16334  -1.19383  -13.53033  L
H-HO-0.427500        0     0.13378  -1.52178  -11.50537  L
N-N--0.415700        0    -3.26934   0.33685  -11.32624  L
C-CT-0.014300        -1   -4.60115  -0.00121  -10.79644  L
C-C-0.597300         0    -5.56919   1.18253  -10.76965  L
O-O--0.567900        0    -6.77445   0.95205  -10.77373  L
C-CT--0.204100       0    -4.42804  -0.69231  -9.43491  L
C-C-0.713000         0    -3.67235  -2.00654  -9.56447  L
O-O--0.593100        0    -3.74376  -2.68571  -10.58222  L
N-N--0.919100        0    -2.91508  -2.38469  -8.56638  L
H-H-0.271900         0    -2.47263   0.30991  -10.70397  L
H-H1-0.104800        0    -5.05489  -0.72522  -11.47512  L
H-HC-0.079700        0    -5.40887  -0.92533  -9.03064  L
H-HC-0.079700        0    -3.91103  -0.0297   -8.73968  L
H-H-0.419600         0    -2.46391  -3.28689  -8.65129  L
H-H-0.419600         0    -2.82221  -1.84441  -7.71177  L
N-N--0.415700        0    -5.06798   2.42106  -10.80714  L
C-CT--0.038900       -1   -5.86512   3.6605   -10.77419  L
C-C-0.597300         0    -6.99987   3.68022  -11.79706  L
O-O--0.567900        0    -8.15135   3.70768  -11.37825  L
C-CT-0.365400        0    -4.98586   4.90997  -10.71161  L
O-OH--0.676100       0    -4.18939   4.76812  -9.54966  L
C-CT--0.243800       0    -5.78792   6.19453  -10.54668  L
H-H-0.271900         0    -4.06121   2.50546  -10.88696  L
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H-H1-0.100700        0    -6.38445   3.64706  -9.81507  L
H-H1-0.004300        0    -4.35456   4.99025  -11.59431  L
H-HC-0.064200        0    -5.11253   7.03698  -10.40088  L
H-HC-0.064200        0    -6.44624   6.11228  -9.68208  L
H-HC-0.064200        0    -6.3909    6.38087  -11.43504  L
H-HO-0.410200        0    -3.513     4.09954  -9.74433  L
N-N--0.254800        0    -6.77067   3.54024  -13.1105  L
C-CT--0.026600       -1   -7.86998   3.45688  -14.07695  L
C-C-0.589600         0    -8.57952   2.08802  -14.17634  L
O-O--0.574800        0    -9.28624   1.83521  -15.14591  L
C-CT--0.007000       0    -7.20115   3.84216  -15.40695  L
C-CT-0.018900        0    -5.78091   3.29965  -15.25449  L
C-CT-0.019200        0    -5.48225   3.59457  -13.78738  L
H-H1-0.064100        0    -8.63126   4.20413  -13.8472  L
H-HC-0.025300        0    -7.16456   4.92995  -15.49002  L
H-HC-0.025300        0    -7.70146   3.42535  -16.28169  L
H-HC-0.021300        0    -5.07909   3.80354  -15.91986  L
H-HC-0.021300        0    -5.77423   2.22205  -15.4255  L
H-H1-0.039100        0    -4.78004   2.86432  -13.39084  L
H-H1-0.039100        0    -5.06766   4.59965  -13.69907  L
N-N--0.347900        0    -8.45111   1.20918  -13.17389  L
C-CT--0.240000       -1   -9.39181   0.09566  -12.91217  L
C-C-0.734100         0    -9.88594   0.14128  -11.45529  L
O-O--0.589400        0    -10.30376  -0.87565  -10.90655  L
C-CT--0.009400       0    -8.77647  -1.27997  -13.24526  L
C-CT-0.018700        0    -8.04914  -1.4135   -14.59291  L
C-CT--0.047900       0    -6.54523  -1.16026  -14.42765  L
C-CT--0.014300       0    -5.79507  -1.42436  -15.7328  L
N-N3--0.385400       0    -4.3357   -1.36862  -15.4929  L
H-H-0.274700         0    -7.82094   1.46223  -12.42005  L
H-H1-0.142600        0    -10.27843   0.22305  -13.53796  L
H-HC-0.036200        0    -9.5907   -2.00709  -13.23971  L
H-HC-0.036200        0    -8.09004  -1.56461  -12.44978  L
H-HC-0.010300        0    -8.47765  -0.73527  -15.33111  L
H-HC-0.010300        0    -8.18227  -2.43557  -14.95089  L
H-HC-0.062100        0    -6.16001  -1.8302   -13.65621  L
H-HC-0.062100        0    -6.37402  -0.13059  -14.11419  L
H-HP-0.113500        0    -6.09642  -0.67407  -16.47046  L
H-HP-0.113500        0    -6.07668  -2.41177  -16.11051  L
H-H-0.340000         0    -4.06305  -2.0784   -14.81037  L
H-H-0.340000         0    -4.09566  -0.48404  -15.04885  L
H-H-0.340000         0    -3.80509  -1.49086  -16.34209  L
N-N--0.415700        0    -9.79785   1.32377  -10.84925  L
C-CT--0.003100       -1   -10.33717   1.73583  -9.55846  L
C-C-0.597300         0    -11.27136   2.95075  -9.80568  L
N-N--0.415700        0    -10.7907   3.98627  -10.51795  L
C-CT--0.149000       -1   -11.54974   5.08887  -11.12597  L
O-O--0.567900        0    -12.43822   2.90197  -9.43037  L
C-CT--0.003600       0    -9.23049   2.0315   -8.54561  L
C-CT--0.064500       0    -8.72773   0.70849  -7.96528  L
C-C-0.695100         0    -7.54464   0.89165  -7.03839  L
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O-O--0.608600        0    -7.32812   1.93515  -6.44066  L
N-N--0.940700        0    -6.71968  -0.1139   -6.88234  L
H-H-0.271900         0    -9.38978   2.06761  -11.39525  L
H-H-0.271900         0    -9.79587   3.97288  -10.70271  L
H-H1-0.085000        0    -10.97311   0.9417   -9.15993  L
H-HC-0.017100        0    -9.63262   2.643    -7.7369   L
H-HC-0.017100        0    -8.41287   2.57294  -9.02018  L
H-HC-0.035200        0    -8.42604   0.0609   -8.78272  L
H-HC-0.035200        0    -9.53381   0.2295   -7.41058  L
H-H-0.425100         0    -6.02237  -0.00529  -6.15353  L
H-H-0.425100         0    -6.89591  -1.02656  -7.28774  L
H-H1-0.097600        0    -11.62632   5.91296  -10.41382  L
H-H1-0.097600        0    -12.55656   4.75249  -11.38229  L
H-H1-0.097600        0    -11.04562   5.4406   -12.02671  L
N-N--0.415700        0    -5.33989   11.36442  -6.79986  L
C-CT--0.002400       -1   -4.38385   10.34545  -6.3701   L
C-C-0.597300         0    -2.93246   10.86332  -6.33869  L
O-O--0.567900        0    -2.6612    11.97936  -6.77326  L
C-CT--0.034300       0    -4.45618   9.13756  -7.32324  L
C-CA-0.011800        0    -5.70633   8.28473  -7.27554  L
C-CA--0.125600       0    -5.71932   7.10148  -6.51005  L
C-CA--0.170400       0    -6.82689   8.62115  -8.0569   L
C-CA--0.107200       0    -6.85124   6.26739  -6.52087  L
C-CA--0.170400       0    -7.95629   7.78785  -8.06271  L
C-CA--0.125600       0    -7.96755   6.60823  -7.29867  L
H-H-0.271900         0    -6.27137   11.07737  -7.07449  L
H-H-0.271900         0    -4.95008   12.24014  -7.13268  L
H-H1-0.097800        0    -4.64743   10.02215  -5.36715  L
H-HC-0.029500        0    -3.62664   8.47302  -7.09175  L
H-HC-0.029500        0    -4.30977   9.48795  -8.34614  L
H-HA-0.133000        0    -4.86691   6.83318  -5.90386  L
H-HA-0.143000        0    -6.83366   9.50316  -8.67839  L
H-HA-0.129700        0    -6.88656   5.37098  -5.92101  L
H-HA--0.170400       0    -8.80398   8.05773  -8.67311  L
H-HA--0.125600       0    -8.82745   5.95519  -7.30344  L
N-N--0.415700        0    -2.00328   10.0296  -5.85869  L
C-CT--0.023700       -1   -0.55355   10.12146  -6.09381  L
C-C-0.597300         0     0.07198   8.73909  -5.91808  L
O-O--0.567900        0    -0.40339   7.94683  -5.10134  L
C-CT-0.034200        0     0.06729   11.11232  -5.09131  L
C-CT-0.001800        0     1.50943   11.50714  -5.42343  L
S-S--0.273700        0     2.23344   12.62831  -4.19719  L
C-CT--0.053600       0     3.72064   13.15817  -5.08629  L
H-H-0.271900         0    -2.32812   9.14522  -5.48509  L
H-H1-0.088000        0    -0.37994   10.47327  -7.1125   L
H-HC-0.024100        0     0.0443    10.67483  -4.09284  L
H-HC-0.024100        0    -0.52435   12.02758  -5.08161  L
H-H1-0.044000        0     1.51798   11.99924  -6.39667  L
H-H1-0.044000        0     2.13393   10.616   -5.47602  L
H-H1-0.068400        0     4.29769   13.83372  -4.45444  L
H-H1-0.068400        0     3.43405   13.68002  -5.99973  L
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H-H1-0.068400        0     4.33062   12.29249  -5.33999  L
N-N--0.415700        0     1.12762   8.45586  -6.67851  L
C-CT--0.058100       -1    1.68372   7.11372  -6.84343  L
C-C-0.597300         0     3.2189    7.17293  -6.76659  L
O-O--0.567900        0     3.91329   7.15642  -7.77956  L
C-CT--0.007400       0     1.18974   6.52867  -8.17804  L
C-CC-0.186800        0    -0.24604   6.84353  -8.4951   L
N-NB--0.543200       0    -0.67303   7.96749  -9.19901  L
C-CW--0.220700       0    -1.32375   6.08373  -8.1624   L
C-CR-0.163500        0    -1.99765   7.84487  -9.32203  L
N-NA--0.279500       0    -2.41533   6.72662  -8.70532  L
H-H-0.271900         0     1.40492   9.14567  -7.36106  L
H-H1-0.136000        0     1.32749   6.45978  -6.04925  L
H-HC-0.036700        0     1.31863   5.44817  -8.15749  L
H-HC-0.036700        0     1.78352   6.92676  -9.00157  L
H-H4-0.186200        0    -1.28847   5.14597  -7.6298   L
H-H-0.333900         0    -3.3679    6.37194  -8.7492   L
H-H5-0.143500        0    -2.62951   8.53783  -9.86299  L
N-N--0.415700        0     3.76278   7.32323  -5.55892  L
C-CT--0.059700       -1    5.17692   7.66294  -5.35084  L
C-C-0.597300         0     6.12613   6.4976   -5.69467  L
O-O--0.567900        0     5.82896   5.34839  -5.35448  L
C-CT-0.130300        0     5.42787   8.20468  -3.91962  L
C-CT--0.043000       0     5.14679   7.18727  -2.78882  L
C-CT--0.320400       0     4.61059   9.49357  -3.71929  L
C-CT--0.066000       0     5.49917   7.69095  -1.38321  L
H-H-0.271900         0     3.13939   7.27654  -4.75941  L
H-H1-0.086900        0     5.37422   8.48538  -6.03055  L
H-HC-0.018700        0     6.48308   8.47786  -3.86196  L
H-HC-0.023600        0     5.72311   6.28465  -2.9706   L
H-HC-0.023600        0     4.09775   6.91249  -2.78952  L
H-HC-0.088200        0     3.54719   9.26645  -3.63233  L
H-HC-0.088200        0     4.76654   10.16977  -4.55823  L
H-HC-0.088200        0     4.93329   10.00419  -2.8126   L
H-HC-0.018600        0     4.79438   8.46241  -1.07415  L
H-HC-0.018600        0     6.51015   8.09763  -1.37087  L
H-HC-0.018600        0     5.43478   6.86328  -0.67655  L
N-N--0.254800        0     7.26808   6.75664  -6.35975  L
C-CT--0.026600       -1    8.09983   5.70638  -6.9409   L
C-C-0.589600         0     8.57669   4.56979  -6.04647  L
O-O--0.574800        0     8.75346   4.75742  -4.84157  L
C-CT--0.007000       0     9.2956    6.42613  -7.56489  L
C-CT-0.018900        0     8.72136   7.77598  -7.96446  L
C-CT-0.019200        0     7.71973   8.05917  -6.84891  L
H-H1-0.064100        0     7.52948   5.27393  -7.75328  L
H-HC-0.025300        0     9.66862   5.88651  -8.43484  L
H-HC-0.025300        0     10.08187   6.56972  -6.82177  L
H-HC-0.021300        0     8.19319   7.68008  -8.91493  L
H-HC-0.021300        0     9.4914    8.54533  -8.02712  L
H-H1-0.039100        0     8.20744   8.60334  -6.03929  L
H-H1-0.039100        0     6.90841   8.65107  -7.27051  L
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N-N--0.415700        0     8.8343    3.40826  -6.6518   L
C-CT--0.051800       -1    9.24582   2.18148  -5.96384  L
C-C-0.597300         0     10.48387   2.36833  -5.05975  L
O-O--0.567900        0     11.52115   2.86445  -5.50153  L
C-CT--0.110200       0     9.4684    1.04574  -6.97171  L
C-CT-0.353100        0     8.24114   0.63475  -7.80562  L
C-CT--0.412100       0     8.59108  -0.57297  -8.67434  L
C-CT--0.412100       0     7.02843   0.27955  -6.94901  L
H-H-0.271900         0     8.66854   3.37817  -7.65928  L
H-H1-0.092200        0     8.42642   1.88943  -5.3132   L
H-HC-0.045700        0     9.80712   0.17317  -6.41317  L
H-HC-0.045700        0     10.26387   1.34863  -7.65271  L
H-HC--0.036100       0     7.95268   1.4428   -8.46409  L
H-HC-0.100000        0     8.93675  -1.39473  -8.05296  L
H-HC-0.100000        0     9.37382  -0.2863   -9.37773  L
H-HC-0.100000        0     7.71766  -0.88176  -9.24809  L
H-HC-0.100000        0     7.28606  -0.47132  -6.2046   L
H-HC-0.100000        0     6.24446  -0.09428  -7.604    L
H-HC-0.100000        0     6.65128   1.17049  -6.44951  L
N-N--0.415700        0     10.38611   1.90918  -3.80419  L
C-CT--0.059700       -1    11.53798   1.46802  -2.99426  L
C-C-0.597300         0     11.8842   0.05763  -3.48226  L
O-O--0.567900        0     11.03654  -0.84192  -3.46785  L
C-CT-0.130300        0     11.21469   1.50405  -1.48447  L
C-CT--0.043000       0     10.75056   2.89738  -0.99455  L
C-CT--0.320400       0     12.42458   1.0295   -0.65986  L
C-CT--0.066000       0     11.6537   4.07843  -1.37599  L
H-H-0.271900         0     9.46971   1.56507  -3.53695  L
H-H1-0.086900        0     12.38655   2.12485  -3.18932  L
H-HC-0.018700        0     10.39732   0.80705  -1.29262  L
H-HC-0.023600        0     10.66889   2.88168   0.09163  L
H-HC-0.023600        0     9.75307   3.08905  -1.38906  L
H-HC-0.088200        0     12.64696  -0.01344  -0.88672  L
H-HC-0.088200        0     12.20424   1.10452   0.40511  L
H-HC-0.088200        0     13.30284   1.63417  -0.88882  L
H-HC-0.018600        0     11.29314   4.98113  -0.88416  L
H-HC-0.018600        0     11.62482   4.2387   -2.4534   L
H-HC-0.018600        0     12.67945   3.89624  -1.0571   L
N-N--0.415700        0     13.10576  -0.11791  -3.97452  L
C-CT--0.051800       -1    13.52823  -1.25735  -4.78169  L
C-C-0.597300         0     14.57634  -2.11696  -4.09105  L
O-O--0.567900        0     15.35219  -1.65321  -3.25872  L
C-CT--0.110200       0     14.09783  -0.76074  -6.133    L
C-CT-0.353100        0     13.13998   0.00428  -7.0615   L
C-CT--0.412100       0     13.93567   0.71056  -8.16008  L
C-CT--0.412100       0     12.16073  -0.94351  -7.74696  L
H-H-0.271900         0     13.71215   0.6961   -3.97505  L
H-H1-0.092200        0     12.66225  -1.88487  -4.9815   L
H-HC-0.045700        0     14.49434  -1.61357  -6.68544  L
H-HC-0.045700        0     14.9393  -0.10913  -5.92276  L
H-HC--0.036100       0     12.58896   0.75057  -6.49725  L
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H-HC-0.100000        0     14.48142  -0.01492  -8.7627   L
H-HC-0.100000        0     14.64157   1.41043  -7.71596  L
H-HC-0.100000        0     13.25416   1.27017  -8.80311  L
H-HC-0.100000        0     11.55467  -0.3848   -8.45866  L
H-HC-0.100000        0     11.51121  -1.39556  -7.00215  L
H-HC-0.100000        0     12.70553  -1.70934  -8.29146  L
N-N--0.415700        0     14.64793  -3.36427  -4.52886  L
C-CT--0.025200       -1    15.75885  -4.25339  -4.27162  L
C-C-0.597300         0     15.76776  -5.48273  -5.18907  L
N-N--0.415700        0     16.54014  -6.50432  -4.80794  L
C-CT--0.149000       0     16.76215  -7.72577  -5.57943  L
O-O--0.567900        0     15.09378  -5.51533  -6.22609  L
H-H-0.271900         0     13.9489  -3.66532  -5.20007  L
H-H-0.271900         0     17.01186  -6.41523  -3.90898  L
H-H1-0.069800        0     15.72242  -4.59239  -3.23765  L
H-H1-0.069800        0     16.69482  -3.71364  -4.41896  L
H-H1-0.097600        0     17.38509  -7.5033   -6.44824  L
H-H1-0.097600        0     15.81162  -8.13637  -5.92146  L
H-H1-0.097600        0     17.27303  -8.46596  -4.96039  L
N-N--0.415700        0     13.73798  -4.20544  -8.60434  L
C-CT--0.038900       -1    12.34491  -4.66992  -8.46828  L
C-C-0.597300         0     11.72189  -4.22463  -7.12997  L
O-O--0.567900        0     12.48753  -3.9452   -6.21027  L
C-CT-0.365400        0     12.28382  -6.20835  -8.57182  L
O-OH--0.676100       0     13.04916  -6.86322  -7.57846  L
C-CT--0.243800       0     12.77464  -6.72226  -9.92404  L
H-H-0.271900         0     14.33511  -4.23495  -7.78101  L
H-H-0.271900         0     14.10224  -3.89098  -9.49456  L
H-H1-0.100700        0     11.75069  -4.2427   -9.27553  L
H-H1-0.004300        0     11.25318  -6.52803  -8.45517  L
H-HC-0.064200        0     12.62026  -7.79986  -9.98061  L
H-HC-0.064200        0     13.83654  -6.51151  -10.05318  L
H-HC-0.064200        0     12.21015  -6.24707  -10.72658  L
H-HO-0.410200        0     13.7622  -6.2625   -7.29152  L
N-N--0.254800        0     10.38435  -4.12976  -6.96431  L
C-CT--0.026600       -1    9.76763  -3.64764  -5.71709  L
C-C-0.589600         0     10.16347  -4.50071  -4.51319  L
O-O--0.574800        0     10.00627  -5.72302  -4.5167   L
C-CT--0.007000       0     8.2539   -3.64291  -5.95777  L
C-CT-0.018900        0     8.07225  -4.62255  -7.11241  L
C-CT-0.019200        0     9.34595  -4.44128  -7.93586  L
H-H1-0.064100        0     10.08717  -2.62117  -5.53312  L
H-HC-0.025300        0     7.93735  -2.65111  -6.27411  L
H-HC-0.025300        0     7.69129  -3.95114  -5.07506  L
H-HC-0.021300        0     7.17466  -4.40841  -7.69348  L
H-HC-0.021300        0     8.04411  -5.63582  -6.71351  L
H-H1-0.039100        0     9.55367  -5.35067  -8.49458  L
H-H1-0.039100        0     9.22582  -3.60426  -8.62408  L
N-N--0.415700        0     10.7074  -3.84305  -3.49087  L
C-CT--0.051800       -1    11.1591  -4.47775  -2.25832  L
C-C-0.597300         0     9.99257  -5.08943  -1.48385  L
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 O-O--0.567900        0     8.91385  -4.49879  -1.4292   L
 C-CT--0.110200       0     11.87426  -3.40447  -1.4152   L
 C-CT-0.353100        0     12.82185  -3.98279  -0.34987  L
 C-CT--0.412100       0     14.14735  -4.40801  -0.98233  L
 C-CT--0.412100       0     13.11304  -2.91898   0.70308  L
 H-H-0.271900         0     10.79268  -2.83583  -3.56306  L
 H-H1-0.092200        0     11.86515  -5.26476  -2.52003  L
 H-HC-0.045700        0     11.11371  -2.78907  -0.93143  L
 H-HC-0.045700        0     12.45473  -2.74969  -2.06639  L
 H-HC--0.036100       0     12.36198  -4.83808   0.1437   L
 H-HC-0.100000        0     14.60772  -3.55598  -1.48086  L
 H-HC-0.100000        0     13.98    -5.20872  -1.70117  L
 H-HC-0.100000        0     14.83868  -4.76392  -0.22209  L
 H-HC-0.100000        0     13.54905  -2.03713   0.23576  L
 H-HC-0.100000        0     13.80666  -3.30689   1.44747  L
 H-HC-0.100000        0     12.18056  -2.64931   1.1975   L
 N-N--0.415700        0     10.2205  -6.25671  -0.8828   L
 C-CT--0.024900       -1    9.25102  -6.9432   -0.03446  L
 C-C-0.597300         0     9.92467  -7.93728   0.92061  L
 O-O--0.567900        0     11.13722  -7.91177   1.14833  L
 C-CT-0.211700        0     8.1867   -7.58193  -0.94621  L
 O-OH--0.654600       0     7.0953   -8.08563  -0.19695  L
 H-H-0.271900         0     11.12121  -6.70658  -1.01234  L
 H-H1-0.084300        0     8.75198  -6.19439   0.5822   L
 H-H1-0.035200        0     8.64149  -8.39227  -1.51804  L
 H-H1-0.035200        0     7.81028  -6.83299  -1.64344  L
 H-HO-0.427500        0     6.31029  -7.50001  -0.29308  L
 N-N--0.347900        0     9.10903  -8.79478   1.52766  L
 C-CT--0.240000       -1    9.44019  -9.83433   2.49739  L
 C-C-0.734100         0     10.36074  -10.91664   1.91756  L
 O-O--0.589400        0     11.32142  -11.30419   2.57609  L
 C-CT--0.009400       0     8.11255  -10.37134   3.09703  L
 C-CT-0.018700        0     7.18228  -9.27306   3.70129  L    H-HC
1455  0.        0.
 C-CT--0.047900       0     5.81312  -9.11385   3.00018  H
 C-CT--0.014300       0     5.04897  -7.84492   3.39524  H
 N-N3--0.385400       0     3.71595  -7.77053   2.72307  H
 H-H-0.274700         0     8.14419  -8.72029   1.22297  L
 H-H1-0.142600        0     10.00954  -9.37332   3.30691  L
 H-HC-0.036200        0     8.36427  -11.07851   3.88912  L
 H-HC-0.036200        0     7.56883  -10.92848   2.33299  L
 H-HC-0.010300        0     7.69505  -8.31016   3.69311  L
 H-HC-0.010300        0     6.99533  -9.51697   4.74819  L
 H-HC-0.062100        0     5.20986  -9.99825   3.23107  H
 H-HC-0.062100        0     5.97607  -9.10605   1.91978  H
 H-HP-0.113500        0     5.59064  -6.94446   3.10699  H
 H-HP-0.113500        0     4.86098  -7.78663   4.46933  H
 H-H-0.340000         0     3.82069  -7.94609   1.71664  H
 H-H-0.340000         0     2.95496  -6.73529   2.8018   H
 H-H-0.340000         0     3.12627  -8.55302   3.04446  H
 N-N--0.347900        0     10.13881  -11.27919   0.64703  L
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C-CT--0.263700       -1    11.06962  -11.86175  -0.35032  L
C-C-0.734100         0     12.56217  -11.58952  -0.11281  L
O-O--0.589400        0     13.38344  -12.45579  -0.38723  L
C-CT--0.000700       0     10.59553  -11.33407  -1.71633  L
C-CT-0.039000        0     11.53201  -11.58023  -2.90903  L
C-CT-0.048600        0     10.86498  -10.99646  -4.15927  L
N-N2--0.529500       0     11.8212   -10.77584  -5.2603   L
C-CA-0.807600        0     11.74243   -9.81818  -6.16958  L
N-N2--0.862700       0     10.76719   -8.9616   -6.20737  L
N-N2--0.862700       0     12.67216   -9.67641  -7.06675  L
H-H-0.274700         0     9.23357   -10.9781   0.29377  L
H-H1-0.156000        0     10.96492   -12.94786  -0.34076  L
H-HC-0.032700        0     10.4495   -10.25493  -1.62985  L
H-HC-0.032700        0     9.62431   -11.78181  -1.93644  L
H-HC-0.028500        0     11.71034   -12.64819  -3.04118  L
H-HC-0.028500        0     12.47988   -11.06744  -2.73983  L
H-H1-0.068700        0     10.42294   -10.04297  -3.87715  L
H-H1-0.068700        0     10.06204   -11.66051  -4.4863   L
H-H-0.345600         0     12.60958   -11.39651  -5.31176  L
H-H-0.447800         0     10.56913   -8.40847  -7.03332  L
H-H-0.447800         0     10.0494   -8.96438  -5.48419  L
H-H-0.447800         0     12.67827   -8.79054  -7.56186  L
H-H-0.447800         0     13.43982   -10.31439  -7.13966  L
N-N--0.415700        0     12.91908   -10.38128   0.31783  L
C-CT--0.058100       -1    14.29441   -9.88022   0.39734  L
C-C-0.597300         0     14.91201   -9.8875    1.80415  L
N-N--0.415700        0     14.19869   -10.39956   2.81531  L
C-CT--0.149000       0     14.66121   -10.5286   4.19487  L
O-O--0.567900        0     16.04224   -9.41855   1.95844  L
C-CT--0.007400       0     14.26118   -8.44841  -0.17113  L
C-CC-0.186800        0     13.71598   -8.28065  -1.57262  L
N-NB--0.543200       0     12.36997   -8.11134  -1.89967  L
C-CW--0.220700       0     14.46246   -8.1035   -2.69993  L
C-CR-0.163500        0     12.33195   -7.84618  -3.21329  L
N-NA--0.279500       0     13.57557   -7.82734  -3.72208  L
H-H-0.271900         0     12.17403   -9.71483   0.46936  L
H-H-0.271900         0     13.2778   -10.76436   2.59028  L
H-H1-0.136000        0     14.94566   -10.48686  -0.23429  L
H-HC-0.036700        0     15.25889   -8.017    -0.14365  L
H-HC-0.036700        0     13.6289   -7.85637   0.48209  L
H-H4-0.186200        0     15.54336   -8.11641  -2.74263  L
H-H-0.333900         0     13.80236   -7.58025  -4.6771   L
H-H5-0.143500        0     11.42846   -7.64154  -3.77333  L
H-H1-0.097600        0     15.38319   -9.74473   4.4288   L
H-H1-0.097600        0     15.14214   -11.4995   4.32779  L
H-H1-0.097600        0     13.81167   -10.45673   4.87555  L
N-N--0.415700        0     14.58703   -6.87344   5.40073  L
C-CT--0.038900       -1    13.90977   -5.68225   4.85584  L
C-C-0.597300         0     12.73934   -5.16221   5.70261  L
O-O--0.567900        0     12.19176   -4.09267   5.41831  L
C-CT-0.365400        0     13.39973   -5.94932   3.43155  L
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O-OH--0.676100       0     12.70055  -7.17664   3.39205  L
C-CT--0.243800       0     14.57602  -6.02015   2.46561  L
H-H-0.271900         0     14.36579  -7.75616   4.95087  L
H-H-0.271900         0     15.38356  -6.78701   6.01911  L
H-H1-0.100700        0     14.62722  -4.86362   4.80817  L
H-H1-0.004300        0     12.73978  -5.14056   3.11505  L
H-HC-0.064200        0     14.19255  -6.05494   1.45371  L
H-HC-0.064200        0     15.18043  -6.90609   2.66074  L
H-HC-0.064200        0     15.197   -5.12984   2.56468  L
H-HO-0.410200        0     12.29741  -7.29226   2.51502  L
N-N--0.415700        0     12.36684  -5.88526   6.7612   L
C-CT--0.024900       -1    11.46314  -5.41178   7.81504  L
C-C-0.597300         0     11.99497  -4.14703   8.48534  L
O-O--0.567900        0     13.19634  -4.04558   8.72201  L
C-CT-0.211700        0     11.28019  -6.50395   8.87114  L
O-OH--0.654600       0     12.54025  -6.95568   9.33093  L
H-H-0.271900         0     12.87992  -6.73432   6.94853  L
H-H1-0.084300        0     10.49915  -5.20212   7.36473  L
H-H1-0.035200        0     10.74004  -7.34355   8.43149  L
H-H1-0.035200        0     10.6994  -6.11226   9.70793  L
H-HO-0.427500        0     13.07124  -6.18487   9.58131  L
N-N--0.415700        0     11.10131  -3.21973   8.83526  L
C-CT--0.087500       -1    11.44337  -1.99701   9.59037  L
C-C-0.597300         0     12.13047  -2.3139    10.92739  L
N-N--0.415700        0     11.62433  -3.31587   11.66495  L
O-O--0.567900        0     13.08215  -1.63103   11.29625  L
C-CT-0.298500        0     10.19654  -1.13549   9.84111  L
C-CT--0.319200       0     10.47873   0.13286   10.65993  L
C-CT--0.319200       0     9.60015  -0.67515   8.51326  L
H-H-0.271900         0     10.1298  -3.41524   8.62072  L
H-H-0.096900         0     10.83312  -3.82394   11.30056  L
H-H1-0.096900        0     12.15603  -1.41492   9.0058   L
H-HC--0.029700       0     9.44849  -1.72945   10.36846  L
H-HC-0.079100        0     9.57778   0.74029   10.73963  L
H-HC-0.079100        0     11.26989   0.7155    10.18642  L
H-HC-0.079100        0     10.7958  -0.13307   11.66887  L
H-HC-0.079100        0     9.31869  -1.52809   7.8986   L
H-HC-0.079100        0     10.31557  -0.05628   7.97256  L
H-HC-0.079100        0     8.71188  -0.09793   8.73829  L
N-N--0.415700        0     14.08549   7.09986   5.628    L
C-CT--0.051800       -1    13.4664   6.44598   4.46715  L
C-C-0.597300         0     12.91484   7.42821   3.41505  L
O-O--0.567900        0     12.6585   7.01662   2.28982  L
C-CT--0.110200       0     12.35066   5.48975   4.93524  L
C-CT-0.353100        0     12.77339   4.38102   5.91874  L
C-CT--0.412100       0     11.55259   3.5364    6.28437  L
C-CT--0.412100       0     13.84287   3.46326   5.32445  L
H-H-0.271900         0     13.58765   7.11731   6.51015  L
H-H-0.271900         0     15.08364   7.27552   5.62383  L
H-H1-0.092200        0     14.22813   5.85522   3.95691  L
H-HC-0.045700        0     11.93223   5.01039   4.05012  L
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H-HC-0.045700        0     11.55781   6.07934   5.39683  L
H-HC--0.036100       0     13.16179   4.83171   6.83203  L
H-HC-0.100000        0     11.83785   2.76665   7.00168  L
H-HC-0.100000        0     11.14389   3.0643    5.39196  L
H-HC-0.100000        0     10.78723   4.1668    6.73682  L
H-HC-0.100000        0     14.02869   2.62788   6.00061  L
H-HC-0.100000        0     14.77671   4.00921   5.19917  L
H-HC-0.100000        0     13.51468   3.07978   4.35871  L
N-N--0.415700        0     12.7473   8.70982   3.75594  L
C-CT-0.033700        0     12.39055   9.77324   2.80902  L
C-C-0.597300         0     13.54193   10.09849   1.83075  L
N-N--0.415700        0     14.75631   10.3169   2.3557   L
C-CT--0.149000       -1    15.97718   10.58998   1.59595  L
O-O--0.567900        0     13.3344   10.14542   0.6194   L
C-CT--0.182500       0     11.95113   11.00899   3.60519  L
H-H-0.271900         0     12.92927   8.96253   4.71342  L
H-H-0.271900         0     14.81813   10.30801   3.36082  L
H-H1-0.082300        0     11.54268   9.43858   2.20709  L
H-HC-0.060300        0     12.76577   11.37414   4.23183  L
H-HC-0.060300        0     11.09418   10.76136   4.23346  L
H-HC-0.060300        0     11.65558   11.80005   2.91351  L
H-H1-0.097600        0     15.73381   10.96944   0.60082  L
H-H1-0.097600        0     16.56574   9.67712   1.501    L
H-H1-0.097600        0     16.57485   11.34388   2.11224  L
N-N--0.415700        0     14.8608   7.13989   0.52716  L
C-CT--0.051800       -1    15.13139   7.83166  -0.72949  L
C-C-0.597300         0     13.86026   8.00922  -1.57562  L
O-O--0.567900        0     12.82206   7.40857  -1.29852  L
C-CT--0.110200       0     16.19756   7.03136  -1.51273  L
C-CT-0.353100        0     17.59723   6.98265  -0.87245  L
C-CT--0.412100       0     18.4605   5.95834  -1.60762  L
C-CT--0.412100       0     18.30405   8.33709  -0.94715  L
H-H-0.271900         0     13.8922   7.13104   0.84806  L
H-H-0.271900         0     15.48843   6.41374   0.83792  L
H-H1-0.092200        0     15.51002   8.8289   -0.51229  L
H-HC-0.045700        0     16.30458   7.45161  -2.51301  L
H-HC-0.045700        0     15.83309   6.00893  -1.62773  L
H-HC--0.036100       0     17.51496   6.67794   0.17106  L
H-HC-0.100000        0     19.4482   5.90783  -1.14854  L
H-HC-0.100000        0     18.57121   6.23688  -2.65605  L
H-HC-0.100000        0     18.0027   4.97004  -1.54998  L
H-HC-0.100000        0     18.4157   8.64789  -1.98659  L
H-HC-0.100000        0     19.29498   8.25705  -0.49845  L
H-HC-0.100000        0     17.74316   9.09379  -0.40484  L
N-N--0.415700        0     13.9638   8.79925  -2.6451   L
C-CT--0.025200       -1    12.95432   8.94091  -3.69754  L
C-C-0.597300         0     12.93395   10.35609  -4.28346  L
N-N--0.415700        0     12.67158   10.47749  -5.58941  L
C-CT--0.149000       0     12.61292   11.75598  -6.29729  L
O-O--0.567900        0     13.1408   11.32267  -3.55113  L
H-H-0.271900         0     14.81679   9.32736  -2.75288  L
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H-H-0.271900          0     12.5249   9.63622  -6.12529  L
H-H1-0.069800         0     11.96323   8.73141  -3.29944  L
H-H1-0.069800         0     13.16343   8.22605  -4.49259  L
H-H1-0.097600         0     11.83814   12.38915  -5.85973  L
H-H1-0.097600         0     12.3895   11.59612  -7.35359  L
H-H1-0.097600         0     13.57134   12.27282  -6.21121  L
N-N--0.415700         0     12.20993   5.46944  -9.56747  L
C-CT--0.025200        -1    12.32941   4.63049  -8.37823  L
C-C-0.597300          0     13.75734   4.59848  -7.82562  L
O-O--0.567900         0     14.67013   5.16542  -8.42422  L
H-H-0.271900          0     11.40542   5.34841  -10.18252  L
H-H-0.271900          0     13.06547   5.86727  -9.93639  L
H-H1-0.069800         0     12.03734   3.61029  -8.62546  L
H-H1-0.069800         0     11.66707   4.99615  -7.59708  L
N-N--0.415700         0     13.95511   3.97743  -6.65927  L
C-CT--0.087500        -1    15.21777   4.03173  -5.89602  L
C-C-0.597300          0     15.50331   2.74169  -5.13038  L
O-O--0.567900         0     14.61681   2.16093  -4.51164  L
C-CT-0.298500         0     15.21611   5.20474  -4.89083  L
C-CT--0.319200        0     15.35023   6.56349  -5.58775  L
C-CT--0.319200        0     13.96413   5.23852  -4.00303  L
H-H-0.271900          0     13.15634   3.51857  -6.22493  L
H-H1-0.096900         0     16.04249   4.18646  -6.59252  L
H-HC--0.029700        0     16.08637   5.09462  -4.24223  L
H-HC-0.079100         0     16.21481   6.55127  -6.25266  L
H-HC-0.079100         0     15.49253   7.34895  -4.84777  L
H-HC-0.079100         0     14.45943   6.78006  -6.17635  L
H-HC-0.079100         0     14.03818   6.05753  -3.30067  L
H-HC-0.079100         0     13.88176   4.31554  -3.43276  L
H-HC-0.079100         0     13.06272   5.36911  -4.60162  L
N-N--0.415700         0     16.75636   2.28908  -5.14733  L
C-CT--0.059700        -1    17.19701   1.07395  -4.44706  L
C-C-0.597300          0     17.40322   1.33608  -2.95704  L
O-O--0.567900         0     17.98254   2.34423  -2.55111  L
C-CT-0.130300         0     18.46445   0.49227  -5.12413  L
C-CT--0.043000        0     18.13871   0.08235  -6.58371  L
C-CT--0.320400        0     19.00637  -0.7263   -4.34921  L
C-CT--0.066000        0     19.36307  -0.30413  -7.42387  L
H-H-0.271900          0     17.45097   2.83239  -5.63618  L
H-H1-0.086900         0     16.41737   0.32186  -4.52487  L
H-HC-0.018700         0     19.23694   1.26371  -5.13709  L
H-HC-0.023600         0     17.66054   0.91442  -7.1001   L
H-HC-0.023600         0     17.43568  -0.75202  -6.57889  L
H-HC-0.088200         0     19.8822  -1.13991  -4.84692  L
H-HC-0.088200         0     18.24076  -1.49913  -4.26971  L
H-HC-0.088200         0     19.32919  -0.43441  -3.34983  L
H-HC-0.018600         0     20.11202   0.48719  -7.37716  L
H-HC-0.018600         0     19.05726  -0.43957  -8.46172  L
H-HC-0.018600         0     19.79513  -1.23945  -7.07001  L
N-N--0.415700         0     16.94059   0.3961   -2.13734  L
C-CT--0.002400        -1    17.22812   0.34974  -0.71684  L
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C-C-0.597300          0     18.68981  -0.07274  -0.44218  L
N-N--0.415700         0     19.60111   0.91081  -0.39062  L
C-CT--0.149000       -1     21.0271    0.74406  -0.08589  L
O-O--0.567900         0     18.98699  -1.25605  -0.28948  L
C-CT--0.034300        0     16.19751  -0.54407  -0.01175  L
C-CA-0.011800         0     16.30532  -0.50223   1.50112  L
C-CA--0.125600        0     15.95262   0.66906   2.20031  L
C-CA--0.125600        0     16.79517  -1.61555   2.20921  L
C-CA--0.170400        0     16.09528   0.72772   3.59892  L
C-CA--0.170400        0     16.92702  -1.56067   3.60832  L
C-CA--0.107200        0     16.57935  -0.38902   4.30307  L
H-H-0.271900          0     16.46149  -0.40064  -2.54433  L
H-H-0.271900          0     19.2682    1.82742  -0.65798  L
H-H1-0.097800         0     17.10664   1.35645  -0.31694  L
H-HC-0.029500         0     16.30831  -1.5717   -0.36251  L
H-HC-0.029500         0     15.19742  -0.21001  -0.28902  L
H-HA-0.133000         0     15.58129   1.52829   1.66168  L
H-HA-0.133000         0     17.09624  -2.506     1.67453  L
H-HA-0.143000         0     15.83817   1.62875   4.13565  L
H-HA-0.143000         0     17.31834  -2.41219   4.14737  L
H-HA-0.129700         0     16.69617  -0.34637   5.37751  L
H-H1-0.097600         0     21.47363   0.03909  -0.79007  L
H-H1-0.097600         0     21.14459   0.34715   0.9243   L
H-H1-0.097600         0     21.54478   1.70139  -0.16066  L
C-CT-0.055800         0    -6.85233  -9.78497  -6.51779  L
C-CT-0.106500         0    -6.24078  -10.88844  -5.65405  L
O-OS--0.354800        0    -5.03099  -11.33275  -6.25025  L
C-CT-0.202200         0    -5.85994  -10.49877  -4.21849  L
O-OS--0.495400        0    -6.91362  -10.47822  -3.26974  L
C-CT-0.067000         0    -4.91725  -11.66608  -3.90783  L
O-OH--0.613900        0    -5.62576  -12.88483  -3.67968  L
C-CT-0.006600         0    -4.15436  -11.80785  -5.22871  L
N-N*--0.048400        0    -2.86619  -11.04739  -5.23433  L
C-C-0.753800          0    -1.70547  -11.69831  -4.80667  L
O-O--0.625800         0    -1.72173  -12.8427  -4.35216  L
N-NC--0.758400        0    -0.50062  -11.03096  -4.90355  L
C-CA--0.521500        0    -0.42207  -9.81904  -5.39502  L
N-N2--0.953800        0     0.76149  -9.3488   -5.66772  L
C-CM--0.521500        0    -1.57     -9.13025  -5.83118  L
C-CM-0.005300         0    -2.7695   -9.76639  -5.7338   L
H-HC-0.067900         0    -7.83187  -9.51071  -6.13913  L
H-HC-0.067900         0    -6.20358  -8.91334  -6.52364  L
H-H1-0.117400         0    -6.93091  -11.73151  -5.61008  L
H-H1-0.061500         0    -5.28548  -9.57233  -4.20826  L
H-H1-0.097200         0    -4.24953  -11.43798  -3.07696  L
H-HO-0.418600         0    -5.79609  -13.00096  -2.71564  L
H-H2-0.202900         0    -3.93255  -12.86908  -5.38147  L
H-H-0.423900          0     1.61461  -9.87176  -5.47066  L
H-H-0.423900          0     0.88513  -8.51507  -6.2405   L
H-HA-0.192800         0    -1.53891  -8.13921  -6.26439  L
H-H4-0.195800         0    -3.6591   -9.2743   -6.0977   L
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 P-P-1.166200         0    -7.62526  -9.13828  -2.80008  L
 O-O2--0.776000       0    -8.38456  -9.51219  -1.5906   L
 O-O2--0.776000       0    -8.38341  -8.60225  -3.94318  L
 O-OS--0.498900       0    -6.45527  -8.10254  -2.42958  L
 C-CT-0.055800        0    -5.61465  -8.22595  -1.28263  L    H-H1
1732  0.        0.
 C-CT-0.106500        0    -4.44001  -7.21647  -1.31112  H
 O-OS--0.354800       0    -3.64992  -7.53956  -2.45356  H
 C-CT-0.202200        0    -4.82709  -5.75461  -1.53935  H
 O-OH--0.654100       0    -5.24118  -5.02206  -0.42909  H
 C-CT-0.067000        0    -3.63448  -5.14398  -2.28673  H
 O-OH--0.613900       0    -2.53141  -4.65116  -1.53763  H
 C-CT-0.039400        0    -3.11246  -6.38433  -3.04746  H
 N-N*--0.025100       0    -3.50134  -6.37699  -4.44187  H
 C-CK-0.200600        0    -4.65058  -6.88932  -5.0027   H
 N-NB--0.607300       0    -4.70402  -6.76447  -6.30169  H
 C-CB-0.051500        0    -3.52672  -6.11676  -6.6188   H
 C-CA-0.700900        0    -2.9234   -5.75317  -7.83797  H
 N-N2--0.901900       0    -3.48932  -6.03974  -9.0397   H
 N-NC--0.761500       0    -1.77726  -5.05543  -7.81092  H
 C-CQ-0.587500        0    -1.19132  -4.84067  -6.62747  H
 N-NC--0.699700       0    -1.58425  -5.23927  -5.41714  H
 C-CB-0.305300        0    -2.77074  -5.85504  -5.4781   H
 H-H1-0.067900        0    -5.20721  -9.2368   -1.22996  L
 H-H1-0.067900        0    -6.21029  -8.04154  -0.39131  L
 H-H1-0.117400        0    -3.85463  -7.30748  -0.38591  H
 H-H1-0.061500        0    -5.57266  -5.76191  -2.32909  H
 H-HO-0.437600        0    -6.16825  -5.2511   -0.21055  H
 H-H1-0.097200        0    -3.9724   -4.36898  -2.98083  H
 H-HO-0.418600        0    -0.8932   -5.72958  -0.3409   H
 H-H2-0.200700        0    -2.02203  -6.38914  -2.98993  H
 H-H5-0.155300        0    -5.40114  -7.35263  -4.38147  H
 H-H-0.411500         0    -2.83366  -6.05392  -9.8086   H
 H-H-0.411500         0    -4.11165  -6.83764  -9.02777  H
 H-H5-0.047300        0    -0.27754  -4.2581   -6.64803  H
 C-CQ-0.587500        0     6.59428   1.8555   -3.10636  L
 P-P-1.166200         0     0.99983  -3.12646   1.24571  H
 N-N3-0.001700        0    -3.78676  -2.98017   0.64562  H
 C-CT-0.058800        0    -3.50894  -2.53478  -0.73122  H
 C-CT-0.090900        0    -3.2732   -1.02194  -0.72617  H
 C-CT--0.023600       0    -2.82732  -0.35935  -2.04284  H
 C-C-0.808700         0    -3.24894   1.10822  -2.01082  H
 O-O2--0.818900       0    -2.50924   1.9269   -1.42903  H
 O-O2--0.818900       0    -4.39034   1.38344  -2.53984  H
 C-C-0.562100         0    -2.33516  -3.31426  -1.29241  H
 O-O--0.588900        0    -1.22639  -2.86771  -1.44291  H
 O-OS--0.421000       0    -0.50924  -3.16949   1.36834  H
 O-O2--0.776000       0     1.56948  -4.04399   0.0948   H
 O-O2--0.776000       0     1.77566  -3.47695   2.53416  H
 O-OS--0.498900       0     1.49318  -1.68683   0.75186  H
 C-CT-0.055800        0     1.21247  -0.59468   1.62578  H
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 C-CT-0.106500        0     1.34584   0.7379    0.86945  L    H-H1
1776  0.        0.
 O-OS--0.354800       0     2.7032    1.0709    0.5914   L
 C-CT-0.039400        0     2.93118   1.06865  -0.81882  L
 N-N*--0.025100       0     4.12705   0.23747  -1.10907  L
 C-CB-0.305300        0     5.22422   0.61805  -1.85205  L
 N-NC--0.699700       0     5.39498   1.77778  -2.54148  L
 N-NC--0.761500       0     7.58309   0.9666   -3.07409  L
 C-CA-0.700900        0     7.35489  -0.17537  -2.42449  L
 N-N2--0.901900       0     8.34897  -1.04522  -2.47098  L
 C-CB-0.051500        0     6.13811  -0.39537  -1.73571  L
 N-NB--0.607300       0     5.63609  -1.4363   -0.94709  L
 C-CK-0.200600        0     4.44467  -1.00573  -0.61463  L
 C-CT-0.067000        0     1.6497    0.59399  -1.50984  L
 O-OH--0.613900       0     1.42819   1.31735  -2.71823  L
 C-CT-0.202200        0     0.56012   0.81831  -0.44278  L
 O-OH--0.654100       0    -0.05594   2.10355  -0.47313  L
 H-H5-0.047300        0     6.79081   2.76328  -3.66     L
 H-H-0.239100         0    -3.07522  -2.60039   1.27839  H
 H-H-0.239100         0    -3.75788  -3.99494   0.73007  H
 H-H-0.239100         0    -5.39662  -2.43048   0.79394  H
 H-HP-0.120200        0    -4.40022  -2.77798  -1.32386  H
 H-HC--0.023200       0    -2.50018  -0.79083   0.00989  H
 H-HC--0.023200       0    -4.22241  -0.59208  -0.3926   H
 H-HC--0.031500       0    -3.26484  -0.85176  -2.91175  H
 H-HC--0.031500       0    -1.74286  -0.41891  -2.13095  H
 H-H1-0.067900        0     1.90356  -0.60368   2.47493  H
 H-H1-0.067900        0     0.18143  -0.67185   1.99545  H
 H-H1-0.117400        0     0.94557   1.5028    1.53204  L
 H-H2-0.200700        0     3.12428   2.086    -1.16978  L
 H-H-0.411500         0     8.17808  -1.98456  -2.14193  L
 H-H-0.411500         0     9.18193  -0.80924  -2.99437  L
 H-H5-0.155300        0     3.76565  -1.57465   0.00511  L
 H-H1-0.097200        0     1.71412  -0.47678  -1.70931  L
 H-HO-0.418600        0     1.94657   0.90097  -3.45558  L
 H-H1-0.061500        0    -0.19722   0.03512  -0.49455  L
 H-HO-0.437600        0    -0.91054   2.01506  -0.95781  L
 O-OW--0.834000       0     6.22244   3.75678  -0.38805  L
 H-HW-0.417000        0     5.26974   3.84259  -0.21062  L
 H-HW-0.417000        0     6.47476   3.07455   0.25915  L
 O-OW--0.834000       0     11.6259   11.08701  -1.2639   L
 H-HW-0.417000        0     12.31235   10.92967  -0.59275  L
 H-HW-0.417000        0     12.12955   11.45186  -2.01137  L
 O-OW--0.834000       0     10.47975   8.67319  -1.1581   L
 H-HW-0.417000        0     10.71275   9.62684  -1.16535  L
 H-HW-0.417000        0     11.35499   8.24918  -1.05913  L
 O-OW--0.834000       0     8.21007   7.25817  -11.86614  L
 H-HW-0.417000        0     7.52723   7.57242  -12.45798  L
 H-HW-0.417000        0     7.81304   6.43106  -11.49693  L
 O-OW--0.834000       0     17.81218  -8.2582    0.16277  L
 H-HW-0.417000        0     18.64633  -8.67721   0.39088  L
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H-HW-0.417000        0     17.20315  -8.61183   0.83727  L
O-OW--0.834000       0     17.45689  -6.49536  -1.94301  L
H-HW-0.417000        0     17.52842  -7.18376  -1.25153  L
H-HW-0.417000        0     17.99167  -5.78462  -1.58091  L
O-OW--0.834000       0     10.27321   2.51993  -10.1666  L
H-HW-0.417000        0     9.3976    2.82794  -9.84415  L
H-HW-0.417000        0     10.47878   3.19569  -10.82496  L
O-OW--0.834000       0     6.35541  -7.83507  -3.55599  L
H-HW-0.417000        0     5.52837  -8.34404  -3.4847   L
H-HW-0.417000        0     6.05718  -6.91516  -3.42531  L
O-OW--0.834000       0     2.3791   -4.40053  -5.42101  L
H-HW-0.417000        0     2.14019  -4.21804  -6.35567  L
H-HW-0.417000        0     2.58115  -3.49646  -5.08493  L
O-OW--0.834000       0     9.95483   5.10776  -11.35938  L
H-HW-0.417000        0     9.06034   4.82577  -11.07313  L
H-HW-0.417000        0     9.74835   5.95211  -11.78712  L
O-OW--0.834000       0    -1.83313  -8.99055  -8.68905  L
H-HW-0.417000        0    -1.17847  -9.62581  -9.00123  L
H-HW-0.417000        0    -1.77344  -9.12056  -7.72761  L
O-OW--0.834000       0    -0.07526  -7.30382  -4.1408   L
H-HW-0.417000        0    -0.65413  -6.77761  -4.70889  L
H-HW-0.417000        0    -0.04999  -8.18234  -4.62935  L
O-OW--0.834000       0     3.87881  -9.01854  -3.49092  L
H-HW-0.417000        0     3.11206  -9.62345  -3.36381  L
H-HW-0.417000        0     3.42952  -8.15806  -3.63119  L
O-OW--0.834000       0     0.32767  -4.37777  -3.47388  L
H-HW-0.417000        0     1.10216  -4.36339  -4.0574   L
H-HW-0.417000        0    -0.36884  -4.72999  -4.0481   L
O-OW--0.834000       0    -0.08742  -5.83195  -0.90203  H
H-HW-0.417000        0    -0.28959  -5.24634  -1.65999  H
H-HW-0.417000        0     0.91681  -4.74382  -0.18945  H
O-OW--0.834000       0     5.46131  -5.25078  -3.54319  L
H-HW-0.417000        0     5.25032  -5.52622  -4.45571  L
H-HW-0.417000        0     5.49708  -4.27439  -3.62956  L
O-OW--0.834000       0    -6.5153   -8.74791   2.03303  L
H-HW-0.417000        0    -6.38538  -7.9227    2.54277  L
H-HW-0.417000        0    -7.16004  -8.48023   1.36247  L
O-OW--0.834000       0     4.73462  -10.42588  -1.06746  L
H-HW-0.417000        0     4.00117  -10.10919  -0.51276  L
H-HW-0.417000        0     4.54587  -10.02166  -1.92617  L
O-OW--0.834000       0     2.51565  -6.7389   -3.91967  L
H-HW-0.417000        0     1.5609   -6.96155  -4.00354  L
H-HW-0.417000        0     2.57507  -5.88822  -4.39202  L
O-OW--0.834000       0     4.75176  -6.78427   0.03238  L
H-HW-0.417000        0     3.92272  -7.02233  -0.42397  L
H-HW-0.417000        0     4.79444  -5.82658  -0.15844  L
O-OW--0.834000       0     4.74904  -6.06303  -6.0712   L
H-HW-0.417000        0     4.42817  -6.98108  -6.16195  L
H-HW-0.417000        0     3.9359   -5.53894  -6.11089  L
O-OW--0.834000       0     3.5103   -5.70734   5.43529  L
H-HW-0.417000        0     2.65864  -5.23105   5.4772   L
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H-HW-0.417000        0     3.38487  -6.45132   6.04683  L
O-OW--0.834000       0     5.20992  -2.60121  -3.62863  L
H-HW-0.417000        0     4.32821  -2.3181   -3.93948  L
H-HW-0.417000        0     5.22851  -2.27592  -2.7144   L
O-OW--0.834000       0     0.63184  -13.93893  -3.55254  L
H-HW-0.417000        0    -0.2559   -13.69068  -3.87728  L
H-HW-0.417000        0     1.20167  -13.6394  -4.28264  L
O-OW--0.834000       0     4.51494  -4.32581  -0.97316  L
H-HW-0.417000        0     4.87318  -4.63394  -1.82389  L
H-HW-0.417000        0     3.71568  -3.82715  -1.2582   L
O-OW--0.834000       0     2.64562  -9.20422   0.3296   L
H-HW-0.417000        0     1.74458  -9.53653   0.42176  L
H-HW-0.417000        0     2.52364  -8.45919  -0.29463  L
O-OW--0.834000       0     0.01103  -10.97598  -7.80391  L
H-HW-0.417000        0    -0.08525  -10.47775  -6.93244  L
H-HW-0.417000        0    -0.49661  -11.76835  -7.61606  L
O-OW--0.834000       0     7.40177  -10.77453  -0.36692  L
H-HW-0.417000        0     7.26101  -9.81473  -0.43232  L
H-HW-0.417000        0     6.52607  -11.10455  -0.63015  L
O-OW--0.834000       0     4.29927  -3.75951   1.74155  L
H-HW-0.417000        0     3.34824  -3.61123   1.89427  L
H-HW-0.417000        0     4.33081  -3.94275   0.78394  L
O-OW--0.834000       0     2.51195  -2.88006  -2.12679  H
H-HW-0.417000        0     1.58413  -3.15353  -2.02694  H
H-HW-0.417000        0     2.49863  -2.46782  -3.03099  H
O-OW--0.834000       0     8.90239  -8.16874  -4.27875  L
H-HW-0.417000        0     7.95171  -8.12307  -4.03332  L
H-HW-0.417000        0     9.15364  -7.22769  -4.32729  L
O-OW--0.834000       0     4.23759  -8.79613  -6.31965  L
H-HW-0.417000        0     3.70771  -9.47221  -6.78812  L
H-HW-0.417000        0     4.21953  -9.10313  -5.39819  L
O-OW--0.834000       0     1.67191  -3.82678  -7.98155  L
H-HW-0.417000        0     1.37922  -2.89763  -8.08052  L
H-HW-0.417000        0     1.32347  -4.24819  -8.77029  L
O-OW--0.834000       0     2.85826  -1.63426   4.52814  H
H-HW-0.417000        0     2.275    -2.22032   4.02155  H
H-HW-0.417000        0     3.63856  -2.21366   4.62807  H
O-OW--0.834000       0     1.76429  -12.36424  -5.50008  L
H-HW-0.417000        0     2.17445  -11.9632  -6.27884  L
H-HW-0.417000        0     0.91975  -11.85267  -5.41206  L
O-OW--0.834000       0     6.67212  -7.78571  -7.3351   L
H-HW-0.417000        0     6.32528  -6.96735  -6.94901  L
H-HW-0.417000        0     5.97897  -8.42017  -7.09077  L
O-OW--0.834000       0     2.36536  -7.05345  -1.24447  L
H-HW-0.417000        0     1.57299  -6.50652  -1.09354  L
H-HW-0.417000        0     2.52718  -6.9102   -2.19852  L
O-OW--0.834000       0     1.7434   -10.57349  -3.34427  L
H-HW-0.417000        0     1.94652  -11.46058  -3.67614  L
H-HW-0.417000        0     0.9728   -10.32887  -3.92017  L
O-OW--0.834000       0    -7.91656  -5.52151   0.10751  L
H-HW-0.417000        0    -8.44247  -4.90339   0.64629  L
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H-HW-0.417000        0    -8.32313  -6.38018   0.30814  L
O-OW--0.834000       0     2.6948   -10.69445  -7.61101  L
H-HW-0.417000        0     2.95836  -11.08714  -8.44819  L
H-HW-0.417000        0     1.71588  -10.64851  -7.69638  L
O-OW--0.834000       0    -3.51986  -2.98289  -13.25932  L
H-HW-0.417000        0    -3.20686  -3.89252  -13.24023  L
H-HW-0.417000        0    -3.61249  -2.78542  -12.30288  L
O-OW--0.834000       0     9.17214  -8.01219  -8.36904  L
H-HW-0.417000        0     8.89264  -8.35418  -9.22116  L
H-HW-0.417000        0     8.31575  -7.90616  -7.89912  L
O-OW--0.834000       0     2.02292  -5.92672   2.76001  H
H-HW-0.417000        0     1.42653  -6.13966   3.49826  H
H-HW-0.417000        0     2.00143  -4.8612    2.67552  H
O-OW--0.834000       0    -0.25777  -8.57825  -0.10306  L
H-HW-0.417000        0    -0.09813  -7.65954  -0.37464  L
H-HW-0.417000        0    -0.52024  -8.99587  -0.94202  L
O-OW--0.834000       0     4.88211  -3.59109   4.40361  L
H-HW-0.417000        0     4.78281  -3.6525    3.4307   L
H-HW-0.417000        0     4.45651  -4.41511   4.71792  L
O-OW--0.834000       0     1.15243  -4.37393   5.14859  H
H-HW-0.417000        0     0.95207  -3.95116   4.29669  H
H-HW-0.417000        0     0.36086  -4.97702   5.221    H
O-OW--0.834000       0    -1.01053  -9.38136  -2.69327  L
H-HW-0.417000        0    -0.75107  -8.47875  -2.94693  L
H-HW-0.417000        0    -0.9264   -9.8205   -3.5856   L
C-CW--0.220700       0     7.99085  -10.50907   10.48598  L
H-H4-0.186200        0     9.03112  -10.38123   10.21625  L
C-CT--0.149000       0     12.17964  -3.74665   12.94345  L
H-H1-0.097600        0     12.14153  -2.92317   13.6586  L
H-H1-0.097600        0     11.6147  -4.59356   13.3333  L
H-H1-0.097600        0     13.22258  -4.04031   12.80817  L
H-HC                 0    -6.9687   -10.14766  -7.53935  L
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**PC**

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N-N--0.347900        0    -7.41584   15.25569   3.86347  L
 C-CT--0.263700       -1   -7.34859   13.89098   4.40682  L
 C-C-0.734100          0    -6.54128   13.01623   3.45067  L
 O-O--0.589400         0    -6.9217    12.88913   2.29335  L
 C-CT--0.000700        0    -8.77302   13.30985   4.56919  L
 C-CT-0.039000         0    -9.55073   13.89425   5.75978  L
 C-CT-0.048600         0    -10.9809   13.32824   5.87969  L
 N-N2--0.529502        0    -11.04406   11.92301   6.34675  L
 C-CA-0.807600         0    -10.96066   11.47859   7.58976  L
 N-N2--0.862702        0    -10.65775   12.25149   8.5955   L
 N-N2--0.862702        0    -11.19504   10.22708   7.84555  L
 H-H-0.274700          0    -7.20376   15.38094   2.87327  L
 H-H-0.274700          0    -7.44936   16.06941   4.46553  L
 H-H1-0.156001         0    -6.84313   13.89812   5.37288  L
 H-HC-0.032700         0    -8.70619   12.22962   4.69513  L
 H-HC-0.032700         0    -9.3369    13.49648   3.65607  L
 H-HC-0.028500         0    -9.62735   14.97394   5.62498  L
 H-HC-0.028500         0    -9.00233   13.70651   6.68323  L
 H-H1-0.068701         0    -11.47268   13.40482   4.90765  L
 H-H1-0.068701         0    -11.54524   13.95752   6.57141  L
 H-H-0.345600          0    -11.33606   11.20906   5.68786  L
 H-H-0.447800          0    -10.62163   11.88283   9.52817  L
 H-H-0.447800          0    -10.51744   13.22991   8.42851  L
 H-H-0.447800          0    -11.16327   9.85301   8.77416  L
 H-H-0.447800          0    -11.5138   9.64561   7.07182  L
 N-N--0.415700         0    -5.46521   12.41187   3.94974  L
 C-CT--0.087500       -1   -4.49498   11.62171   3.17768  L
 C-C-0.597300          0    -4.37234   10.21726   3.74913  L
 O-O--0.567900         0    -4.34166   10.06355   4.97224  L
 C-CT-0.298500         0    -3.15581   12.37535   3.06687  L
 C-CT--0.319200        0    -2.49129   12.61592   4.42419  L
 C-CT--0.319200        0    -2.18817   11.65986   2.12276  L
 H-H-0.271900          0    -5.25302   12.53483   4.92643  L
 H-H1-0.096900         0    -4.87896   11.50869   2.16563  L
 H-HC--0.029700        0    -3.36258   13.35456   2.63384  L
 H-HC-0.079100         0    -3.1505    13.17378   5.08593  L
 H-HC-0.079100         0    -1.58239   13.20243   4.28113  L
 H-HC-0.079100         0    -2.22176   11.66875   4.88964  L
 H-HC-0.079100         0    -1.26504   12.2354   2.04201  L
 H-HC-0.079100         0    -2.63481   11.58117   1.13227  L
 H-HC-0.079100         0    -1.95073   10.66479   2.49151  L
 N-N--0.347900         0    -4.38675   9.19108   2.88356  L
 C-CT--0.263700       -1   -4.58045   7.79981   3.32618  L
 C-C-0.734100          0    -3.43087   6.8317    3.11759  L
 O-O--0.589400         0    -2.51234   7.08362   2.34941  L
 C-CT--0.000700        0    -5.95714   7.22471   2.92498  L
 C-CT-0.039000         0    -6.0253    6.15605   1.81738  L    H-H1
48    0.        0.
 C-CT-0.048600         0    -5.38745   6.56614   0.48816  H
 N-N2--0.529500        0    -5.6718    5.60765  -0.56921  H
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 C-CA-0.807600        0    -4.99447   4.46259  -0.80253  H
 N-N2--0.862700       0    -3.71018   4.32893  -0.44675  H
 N-N2--0.862700       0    -5.63208   3.44919  -1.36777  H
 H-H-0.274700         0    -4.38095   9.41295   1.89526  L
 H-H1-0.156000        0    -4.63057   7.84008   4.41469  L
 H-HC-0.032700        0    -6.6169    8.04402   2.67063  L
 H-HC-0.032700        0    -6.3886    6.76212   3.81437  L
 H-HC-0.028500        0    -7.07903   5.94317   1.63936  L
 H-HC-0.028500        0    -5.56645   5.22935   2.16199  L
 H-H1-0.068700        0    -4.3115    6.67366   0.60408  H
 H-H1-0.068700        0    -5.78761   7.53041   0.19299  H
 H-H-0.345600         0    -6.65854   5.50409  -0.83444  H
 H-H-0.447800         0    -3.2235    3.48606  -0.80415  H
 H-H-0.447800         0    -3.16003   5.18971  -0.39522  H
 H-H-0.447800         0    -5.14438   2.62345  -1.81621  H
 H-H-0.447800         0    -6.6372    3.63129  -1.51993  H
 N-N--0.415700        0    -3.51588   5.70553   3.81256  L
 C-CT--0.002400      -1    -2.58966   4.59229   3.74725  L
 C-C-0.597300         0    -3.29638   3.26885   4.05934  L
 O-O--0.567900        0    -4.08045   3.18921   5.00519  L
 C-CT--0.034300       0    -1.451     4.89276   4.74008  L
 C-CA-0.011800        0    -0.4839    3.76133   5.03743  L
 C-CA--0.125600       0     0.34187   3.22743   4.03021  L
 C-CA--0.125600       0    -0.38788   3.26203   6.34891  L
 C-CA--0.170400       0     1.25383   2.2       4.34044  L
 C-CA--0.170400       0     0.50932   2.22381   6.65292  L
 C-CA--0.107200       0     1.33387   1.6925    5.64713  L
 H-H-0.271900         0    -4.23543   5.65318   4.52562  L
 H-H1-0.097800        0    -2.17004   4.5296    2.74161  L
 H-HC-0.029500        0    -1.89812   5.21522   5.68245  L
 H-HC-0.029500        0    -0.87355   5.73578   4.35764  L
 H-HA-0.133000        0     0.28375   3.61331   3.02356  L
 H-HA-0.133000        0    -1.01609   3.67424   7.12252  L
 H-HA-0.143000        0     1.91544   1.79369   3.58906  L
 H-HA-0.143000        0     0.55691   1.82844   7.65536  L
 H-HA-0.129700        0     2.03346   0.89609   5.86903  L
 N-N--0.415700        0    -3.02439   2.23925   3.25274  L
 C-CT-0.033700       -1    -3.81662   1.01005   3.20144  L
 C-C-0.597300         0    -2.96612  -0.2807    3.34822  L
 O-O--0.567900        0    -2.86452  -1.07606   2.41419  L
 C-CT--0.182500       0    -4.63782   1.08533   1.9078   L
 H-H-0.271900         0    -2.3755    2.39076   2.49636  L
 H-H1-0.082300        0    -4.53383   1.00362   4.02022  L
 H-HC-0.060300        0    -3.97711   1.19875   1.04841  L
 H-HC-0.060300        0    -5.31758   1.93794   1.94657  L
 H-HC-0.060300        0    -5.22624   0.18027   1.79258  L
 N-N--0.254800        0    -2.3287   -0.5445    4.50253  L
 C-CT--0.026600       0    -1.53507  -1.75532   4.72253  L    H-H2
98    0.        0.
 C-C-0.589600         0    -2.36952  -3.06107   4.62077  H
 O-O--0.574800        0    -3.34116  -3.32159   5.30858  H
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 C-CT--0.007000       0    -0.89223  -1.58451   6.10545  L
 C-CT-0.018900        0    -1.77784  -0.54985   6.79486  L
 C-CT-0.019200        0    -2.19537   0.34613   5.63834  L
 H-H1-0.064100        0    -0.73657  -1.7873    3.98037  L
 H-HC-0.025300        0     0.11535  -1.18163   5.99024  L
 H-HC-0.025300        0    -0.86392  -2.51897   6.66699  L
 H-HC-0.021300        0    -1.2467    0.00156   7.57008  L
 H-HC-0.021300        0    -2.66044  -1.04112   7.19944  L
 H-H1-0.039100        0    -3.10895   0.8841    5.87646  L
 H-H1-0.039100        0    -1.40685   1.05565   5.41204  L
 N-N--0.415700        0    -1.86152  -3.92574   3.69595  H
 C-CT--0.024900       0    -2.33627  -5.28814   3.53835  H
 C-C-0.597300         0    -1.88015  -6.12776   4.74395  L    H-H1
111   0.        0.
 O-O--0.567900        0    -0.6795   -6.15816   5.02729  L
 C-CT-0.211700        0    -1.74991  -5.93782   2.29025  H
 O-OH--0.654600       0    -2.06302  -5.2668    1.08164  H
 H-H-0.271900         0    -1.19736  -3.57578   3.01274  H
 H-H1-0.084300        0    -3.4258   -5.28168   3.47218  H
 H-H1-0.035200        0    -2.15353  -6.95007   2.21098  H
 H-H1-0.035200        0    -0.65628  -6.01523   2.38137  H
 H-HO-0.427500        0    -1.61912  -4.39071   1.15299  H
 N-N--0.254800        0    -2.78365  -6.8091    5.47238  L
 C-CT--0.026600       0    -2.45362  -7.65999   6.61079  L
 C-C-0.589600         0    -1.90422  -9.00518   6.11208  L
 O-O--0.574800        0    -2.47197  -10.0667   6.35001  L
 C-CT--0.007000       0    -3.76676  -7.79144   7.38709  L
 C-CT-0.018900        0    -4.81614  -7.77852   6.28169  L
 C-CT-0.019200        0    -4.20987  -6.85635   5.22757  L
 H-H1-0.064100        0    -1.70771  -7.17774   7.24182  L
 H-HC-0.025300        0    -3.89672  -6.91375   8.01578  L
 H-HC-0.025300        0    -3.82058  -8.69421   7.9965   L
 H-HC-0.021300        0    -5.7607   -7.38355   6.64619  L
 H-HC-0.021300        0    -4.94275  -8.78104   5.87011  L
 H-H1-0.039100        0    -4.40249  -7.25566   4.2319   L
 H-H1-0.039100        0    -4.62583  -5.8562    5.33337  L
 N-N--0.415700        0    -0.77671  -8.94074   5.41245  L
 C-CT--0.038900      -1    -0.18085  -10.02262   4.63174  L
 C-C-0.597300         0     1.34253  -10.0636   4.86522  L
 O-O--0.567900        0     2.1492   -9.86224   3.95717  L
 C-CT-0.365400        0    -0.51395  -9.88357   3.13145  L
 O-OH--0.676100       0    -0.22677  -8.57906   2.67286  L
 C-CT--0.243800       0    -1.98982  -10.14466   2.82997  L
 H-H-0.271900         0    -0.40607  -8.01507   5.23693  L
 H-H1-0.100700        0    -0.5755   -10.98377   4.96574  L
 H-H1-0.004300        0     0.07993  -10.60309   2.56634  L
 H-HC-0.064200        0    -2.6171   -9.3977    3.31539  L
 H-HC-0.064200        0    -2.26736  -11.13512   3.19062  L
 H-HC-0.064200        0    -2.15505  -10.10327   1.75317  L
 H-HO-0.410200        0    -0.25766  -8.61188   1.69476  L
 N-N--0.415700        0     1.76226  -10.29961   6.11292  L
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C-CT--0.025200       -1    3.17158  -10.37874   6.52773  L
C-C-0.597300         0     3.75367  -9.08781   7.14317  L
O-O--0.567900        0     3.15312  -8.01199   7.0723   L
H-H-0.271900         0     1.05608  -10.46944   6.81528  L
H-H1-0.069800        0     3.78509  -10.63419   5.66332  L
H-H1-0.069800        0     3.28448  -11.19032   7.24136  L
N-N--0.415700        0     4.94744  -9.20537   7.74431  L
C-CT--0.058100       -1    5.6977   -8.14994   8.46111  L
C-C-0.597300         0     5.92089  -6.88477   7.61288  L
O-O--0.567900        0     6.23933  -6.96565   6.42744  L
C-CT--0.007400       0     7.04697  -8.71135   8.9369   L
C-CC-0.186800        0     6.95103  -9.8199    9.95906  L
N-NB--0.543200       0     5.78148  -10.27672   10.57092  L
C-CR-0.163500        0     6.16612  -11.2299   11.43348  L
N-NA--0.279500       0     7.49973  -11.39776   11.38483  L
H-H-0.271900         0     5.34813  -10.13009   7.77948  L
H-H1-0.136000        0     5.12037  -7.86669   9.34124  L
H-HC-0.036700        0     7.62288  -7.90038   9.38471  L
H-HC-0.036700        0     7.60496  -9.07769   8.07368  L
H-H-0.333900         0     8.02712  -12.05283   11.94826  L
H-H5-0.143500        0     5.49676  -11.7805   12.08255  L
N-N--0.415700        0     5.78531  -5.71883   8.25456  L
C-CT--0.051800       0     5.99511  -4.38209   7.68509  L
C-C-0.597300         0     7.42082  -4.20196   7.14166  L
O-O--0.567900        0     8.38339  -4.29445   7.90938  L
C-CT--0.110200       0     5.72552  -3.35325   8.80135  L
C-CT-0.353100        0     5.97667  -1.88254   8.41342  L
C-CT--0.412100       0     4.95316  -1.34547   7.41591  L
C-CT--0.412100       0     5.92755  -1.02011   9.67211  L
H-H-0.271900         0     5.55153  -5.76582   9.23129  L
H-H1-0.092200        0     5.28503  -4.2288    6.87093  L
H-HC-0.045700        0     6.38008  -3.59459   9.64097  L
H-HC-0.045700        0     4.70074  -3.45946   9.14508  L
H-HC--0.036100       0     6.96651  -1.77707   7.9786   L
H-HC-0.100000        0     3.94802  -1.4054    7.82285  L
H-HC-0.100000        0     5.00386  -1.91549   6.48899  L
H-HC-0.100000        0     5.16823  -0.3052    7.18641  L
H-HC-0.100000        0     4.94463  -1.0959    10.13458  L
H-HC-0.100000        0     6.13545   0.01665   9.41424  L
H-HC-0.100000        0     6.68514  -1.35822   10.37926  L
N-N--0.415700        0     7.55401  -3.84171   5.8622   L
C-CT--0.058100       -1    8.84272  -3.48623   5.25162  L
C-C-0.597300         0     8.97477  -1.98092   5.0143   L
O-O--0.567900        0     8.00158  -1.22195   5.0444   L
C-CT--0.007400       0     9.09094  -4.32781   3.98651  L
C-CC-0.186800        0     8.57982  -3.72179   2.7072   L
N-NB--0.543200       0     9.33821  -2.92999   1.84643  L
C-CW--0.220700       0     7.33602  -3.89334   2.18118  L
C-CR-0.163500        0     8.53599  -2.66616   0.80469  L
N-NA--0.279500       0     7.31983  -3.20233   0.98935  L
H-H-0.271900         0     6.71057  -3.73522   5.30726  L
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H-H1-0.136000        0     9.63826  -3.74862   5.94721  L
H-HC-0.036700        0     8.66116  -5.32268   4.11355  L
H-HC-0.036700        0     10.16495  -4.46045   3.86515  L
H-H4-0.186200        0     6.53434  -4.47947   2.60634  L
H-H-0.333900         0     6.54957  -3.12822   0.32555  L
H-H5-0.143500        0     8.8343   -2.11945  -0.07802  L
N-N--0.415700        0     10.21345  -1.54463   4.80552  L
C-CT--0.087500       -1    10.59554  -0.13325   4.66633  L
C-C-0.597300         0     9.84775   0.62825   3.57232  L
O-O--0.567900        0     9.51636   1.7882    3.7875   L
C-CT-0.298500        0     12.11987   0.01417   4.49922  L
C-CT--0.319200       0     12.84139  -0.36919   5.79711  L
C-CT--0.319200       0     12.68592  -0.82981   3.35183  L
H-H-0.271900         0     10.94824  -2.24487   4.80566  L
H-H1-0.096900        0     10.33081   0.36745   5.59656  L
H-HC--0.029700       0     12.34187   1.05954   4.29199  L
H-HC-0.079100        0     12.68129  -1.42212   6.0326   L
H-HC-0.079100        0     12.47663   0.24159   6.62219  L
H-HC-0.079100        0     13.9119   -0.1971    5.68634  L
H-HC-0.079100        0     12.50056  -1.89041   3.52134  L
H-HC-0.079100        0     13.76185  -0.68582   3.28672  L
H-HC-0.079100        0     12.244    -0.52533   2.40512  L
N-N--0.415700        0     9.54505   0.01633   2.42456  L
C-CT--0.025200       -1    8.75224   0.64608   1.36128  L
C-C-0.597300         0     7.3132    0.94667   1.79384  L
O-O--0.567900        0     6.83534   2.06178   1.58814  L
H-H-0.271900         0     9.7869   -0.96656   2.33968  L
H-H1-0.069800        0     8.72619   0.00891   0.48002  L
H-H1-0.069800        0     9.21834   1.58807   1.08339  L
N-N--0.415700        0     6.6367   -0.01519   2.42759  L
C-CT--0.025200       0     5.32767   0.1786    3.06249  L
C-C-0.597300         0     5.34205   1.29048   4.12054  L
O-O--0.567900        0     4.5761    2.25281   4.04453  L
H-H-0.271900         0     7.09532  -0.90779   2.55898  L
H-H1-0.069800        0     5.0293   -0.75204   3.54141  L
H-H1-0.069800        0     4.58767   0.42759   2.3026   L
N-N--0.415700        0     6.25529   1.19554   5.09222  L
C-CT-0.033700        -1    6.46516   2.20403   6.13883  L
C-C-0.597300         0     6.77667   3.59963   5.58031  L
O-O--0.567900        0     6.29837   4.59788   6.11339  L
C-CT--0.182500       0     7.57297   1.71189   7.06143  L
H-H-0.271900         0     6.84559   0.36802   5.08389  L
H-H1-0.082300        0     5.54189   2.2841    6.71155  L
H-HC-0.060300        0     7.2961    0.72521   7.41957  L
H-HC-0.060300        0     7.68431   2.39144   7.90708  L
H-HC-0.060300        0     8.51709   1.64881   6.51916  L
N-N--0.347900        0     7.56286   3.68661   4.50377  L
C-CT--0.263700       -1    7.8221    4.9234    3.76288  L
C-C-0.734100         0     6.54229   5.57551   3.22684  L
O-O--0.589400        0     6.46152   6.79436   3.29605  L
C-CT--0.000700       0     8.93804   4.681     2.73163  L
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C-CT-0.039000        0     9.23913   5.8359    1.75814  L
C-CT-0.048600        0     8.31253   5.72275   0.54678  L
N-N2--0.529500       0     8.77561   6.47261  -0.62312  L
C-CA-0.807600        0     8.6467    6.07941  -1.87416  L
N-N2--0.862700       0     7.9473    5.04455  -2.2279   L
N-N2--0.862700       0     9.24504   6.72589  -2.82197  L
H-H-0.274700         0     7.98782   2.82686   4.16712  L
H-H1-0.156000        0     8.21652   5.64716   4.47457  L
H-HC-0.032700        0     8.72095   3.77695   2.16447  L
H-HC-0.032700        0     9.85004   4.47882   3.29129  L
H-HC-0.028500        0     10.26926   5.73023   1.41453  L
H-HC-0.028500        0     9.12759   6.80467   2.24694  L
H-H1-0.068700        0     7.3022    6.04143   0.80216  L
H-H1-0.068700        0     8.3021    4.67034   0.27378  L
H-H-0.345600         0     9.31263   7.32542  -0.49809  L
H-H-0.447800         0     7.93683   4.793    -3.20826  L
H-H-0.447800         0     7.34763   4.57578  -1.5517   L
H-H-0.447800         0     9.23541   6.31422  -3.7451   L
H-H-0.447800         0     9.79189   7.53442  -2.55053  L
N-N--0.415700        0     5.53535   4.82833   2.76101  L
C-CT--0.038900      -1     4.20161   5.39212   2.43641  L
C-C-0.597300         0     3.5659    6.05038   3.65974  L
O-O--0.567900        0     3.10691   7.1829    3.56331  L
C-CT-0.365400        0     3.23426   4.34297   1.86735  L
O-OH--0.676100       0     3.8537    3.59714   0.85357  L
C-CT--0.243800       0     2.00101   4.97472   1.22365  L
H-H-0.271900         0     5.66582   3.82571   2.69921  L
H-H1-0.100700        0     4.3362    6.16642   1.68025  L
H-H1-0.004300        0     2.92392   3.66527   2.65944  L
H-HC-0.064200        0     1.43008   5.52861   1.96803  L
H-HC-0.064200        0     1.36729   4.19665   0.79811  L
H-HC-0.064200        0     2.30702   5.65777   0.43002  L
H-HO-0.410200        0     3.42416   2.72571   0.84064  L
N-N--0.415700        0     3.55192   5.37212   4.81513  L
C-CT-0.033700       -1     3.09281   5.95758   6.08025  L
C-C-0.597300         0     3.84595   7.24686   6.42928  L
O-O--0.567900        0     3.209     8.2635    6.6601   L
C-CT--0.182500       0     3.14714   4.91338   7.19374  L
H-H-0.271900         0     3.94806   4.44098   4.82174  L
H-H1-0.082300        0     2.04757   6.23667   5.94751  L
H-HC-0.060300        0     2.59293   4.02802   6.88832  L
H-HC-0.060300        0     2.69725   5.3281    8.09616  L
H-HC-0.060300        0     4.17636   4.64004   7.40675  L
N-N--0.415700        0     5.18111   7.2193    6.43218  L
C-CT--0.051800      -1     6.0499    8.37837   6.66162  L
C-C-0.597300         0     5.74381   9.55046   5.73395  L
O-O--0.567900        0     5.56436   10.6689   6.20122  L
C-CT--0.110200       0     7.51635   7.91518   6.54183  L
C-CT-0.353100        0     8.56916   9.01081   6.80005  L
C-CT--0.412100       0     8.57743   9.46664   8.25894  L
C-CT--0.412100       0     9.96079   8.46919   6.46031  L
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H-H-0.271900          0      5.61219   6.32134   6.24268  L
H-H1-0.092200         0      5.87473   8.72771   7.68009  L
H-HC-0.045700         0      7.66843   7.53673   5.53304  L
H-HC-0.045700         0      7.68547   7.09147   7.23713  L
H-HC--0.036100        0      8.37817   9.86949   6.15757  L
H-HC-0.100000         0      9.3545    10.21624   8.40831  L
H-HC-0.100000         0      8.75735   8.62143   8.9227   L
H-HC-0.100000         0      7.62078   9.92309   8.51056  L
H-HC-0.100000         0      10.18622   7.60635   7.08701  L
H-HC-0.100000         0      10.70248   9.24873   6.63343  L
H-HC-0.100000         0      9.99047   8.18071   5.40962  L
N-N--0.415700         0      5.71421   9.29199   4.43018  L
C-CT--0.002400        -1     5.42822   10.28406   3.40521  L
C-C-0.597300          0      4.04442   10.91504   3.58556  L
O-O--0.567900         0      3.91183   12.13402   3.62073  L
C-CT--0.034300        0      5.5965    9.63515   2.01847  L
C-CA-0.011800         0      5.66005   10.60686   0.85279  L
C-CA--0.125600        0      6.90614   10.95935   0.2971   L
C-CA--0.125600        0      4.48026   11.14066   0.29989  L
C-CA--0.170400        0      6.97154   11.84166  -0.79645  L
C-CA--0.170400        0      4.54435   12.02417  -0.79236  L
C-CA--0.107200        0      5.7902    12.37651  -1.33981  L
H-H-0.271900          0      5.88027   8.33881   4.12942  L
H-H1-0.097800         0      6.1573    11.09082   3.49334  L
H-HC-0.029500         0      4.78348   8.92784   1.84613  L
H-HC-0.029500         0      6.5248    9.06333   2.0162   L
H-HA-0.133000         0      7.82007   10.55639   0.70795  L
H-HA-0.133000         0      3.51794   10.87931   0.71364  L
H-HA-0.143000         0      7.931     12.11504  -1.21363  L
H-HA-0.143000         0      3.63343   12.43286  -1.20825  L
H-HA-0.129700         0      5.83751   13.06126  -2.17472  L
N-N--0.415700         0      3.01371   10.07989   3.71469  L
C-CT-0.014300         -1     1.6306    10.51754   3.86258  L
C-C-0.597300          0      1.32128   11.09996   5.27215  L
O-O--0.567900         0      0.31909   11.79115   5.42838  L
C-CT--0.204100        0      0.69229   9.35212   3.48533  L
C-C-0.713000          0      0.77304   8.94854   2.01551  L
O-O--0.593100         0      1.51387   9.47888   1.20869  L
N-N--0.919100         0     -0.01209   7.99727   1.57799  L
H-H-0.271900          0      3.20029   9.08583   3.65046  L
H-H1-0.104800         0      1.454     11.33359   3.15832  L
H-HC-0.079700         0     -0.3325    9.64322   3.70225  L
H-HC-0.079700         0      0.93532   8.48576   4.09522  L
H-H-0.419600          0      0.10117   7.79764   0.60353  L
H-H-0.419600          0     -0.78082   7.60397   2.10675  L
N-N--0.415700         0      2.12896   10.81745   6.30378  L
C-CT--0.027500        -1     2.14846   11.49518   7.61728  L
C-C-0.597300          0      2.79853   12.88986   7.50815  L
N-N--0.415700         0      3.99673   12.9735   6.91008  L
C-CT--0.149000        -1     4.78331   14.18863   6.69909  L
O-O--0.567900         0      2.21163   13.8693   7.96494  L
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C-CT--0.005000       0     2.87759   10.60752   8.63516  L
C-C*--0.141500       0     3.20243   11.24068   9.95188  L
C-CW--0.163800       0     2.3442    11.41644   10.98189  L
C-CB-0.124300        0     4.47835   11.80484   10.38545  L
N-NA--0.341800       0     3.00387   12.04015   12.02611  L
C-CN-0.138000        0     4.323     12.29573   11.71475  L
C-CA--0.238700       0     5.74794   11.95986   9.78629  L
C-CA--0.260100       0     5.37523   12.89601   12.4225  L
C-CA--0.197200       0     6.81258   12.56144   10.48562  L
C-CA--0.113400       0     6.62943   13.02636   11.80083  L
H-H-0.271900         0     2.85587   10.1328   6.13619  L
H-H-0.271900         0     4.38721   12.10696   6.55774  L
H-H1-0.112300        0     1.12653   11.65068   7.96045  L
H-HC-0.033900        0     3.82035   10.27921   8.19972  L
H-HC-0.033900        0     2.27268   9.71797   8.81605  L
H-H4-0.206200        0     1.30304   11.1214   10.97067  L
H-H-0.341200         0     2.56737   12.31179   12.8946  L
H-HA-0.170000        0     5.88647   11.62809   8.76767  L
H-HA-0.157200        0     5.22004   13.26368   13.42542  L
H-HA-0.144700        0     7.77335   12.68152   10.00466  L
H-HA-0.141700        0     7.44915   13.49702   12.32686  L
H-H1-0.097600        0     5.26199   14.48262   7.63449  L
H-H1-0.097600        0     4.12849   14.99571   6.36533  L
H-H1-0.097600        0     5.54315   14.00713   5.93795  L
N-N--0.415700        0    -3.72865   12.23472   8.5016   L
C-CT--0.002400      -1    -3.36338   10.86617   8.13829  L
C-C-0.597300         0    -4.47964   9.87445   8.49051  L
O-O--0.567900        0    -5.15278   10.0312   9.50862  L
C-CT--0.034300       0    -2.04672   10.52188   8.84761  L
C-CA-0.011800        0    -1.48171   9.15522   8.51504  L
C-CA--0.125600       0    -0.92755   8.91514   7.24434  L
C-CA--0.125600       0    -1.47792   8.13306   9.48345  L
C-CA--0.170400       0    -0.35975   7.66401   6.94884  L
C-CA--0.170400       0    -0.90295   6.88411   9.18924  L
C-CA--0.107200       0    -0.34012   6.65108   7.92254  L
H-H-0.271900         0    -4.40721   12.32936   9.24808  L
H-H-0.271900         0    -3.05485   12.97183   8.33419  L
H-H1-0.097800        0    -3.19087   10.82705   7.06295  L
H-HC-0.029500        0    -2.19772   10.59378   9.92614  L
H-HC-0.029500        0    -1.2978    11.26722   8.57353  L
H-HA-0.133000        0    -0.91577   9.70019   6.50141  L
H-HA-0.133000        0    -1.89777   8.31133   10.46342  L
H-HA-0.143000        0     0.08344   7.49174   5.98037  L
H-HA-0.143000        0    -0.88011   6.1133    9.94553  L
H-HA-0.129700        0     0.12156   5.70158   7.69915  L
N-N--0.415700        0    -4.69967   8.87914   7.63065  L
C-CT--0.059700      -1    -5.70969   7.82777   7.78366  L
C-C-0.597300         0    -5.05937   6.47118   7.49965  L
O-O--0.567900        0    -4.45499   6.30463   6.44036  L
C-CT-0.130300        0    -6.9358    8.07408   6.86645  L
C-CT--0.043000       0    -7.73338   9.35069   7.23133  L
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C-CT--0.320400       0    -7.90505   6.87865   6.96006  L
C-CT--0.066000       0    -7.24576   10.63816   6.55583  L
H-H-0.271900         0    -4.14117   8.86772   6.78498  L
H-H1-0.086900        0    -6.05796   7.81678   8.8172   L
H-HC-0.018700        0    -6.60267   8.1506    5.83078  L
H-HC-0.023600        0    -7.73622   9.48626   8.31366  L
H-HC-0.023600        0    -8.76826   9.22287   6.91516  L
H-HC-0.088200        0    -8.21752   6.71645   7.99245  L
H-HC-0.088200        0    -7.4421    5.96787   6.5777   L
H-HC-0.088200        0    -8.78847   7.05501   6.34947  L
H-HC-0.018600        0    -6.24844   10.91043   6.88506  L
H-HC-0.018600        0    -7.92096   11.45057   6.81879  L
H-HC-0.018600        0    -7.23884   10.50861   5.4746   L
N-N--0.415700       -1    -5.20785   5.50253   8.41486  L
C-CT--0.051800       0    -4.61888   4.16982   8.28287  L
C-C-0.597300         0    -5.73621   3.13222   8.28275  L
O-O--0.567900        0    -6.46216   3.00304   9.26778  L
C-CT--0.110200       0    -3.57525   3.95364   9.39713  L
C-CT-0.353100        0    -2.7656    2.64279   9.27248  L
C-CT--0.412100       0    -1.41519   2.79489   9.98019  L
C-CT--0.412100       0    -3.45403   1.4271    9.89849  L
H-H-0.271900         0    -5.76128   5.68615   9.23802  L
H-H1-0.092200        0    -4.09416   4.09959   7.32981  L
H-HC-0.045700        0    -4.06063   3.99276   10.37363  L
H-HC-0.045700        0    -2.8803    4.79118   9.34118  L
H-HC--0.036100       0    -2.57729   2.4311    8.22072  L
H-HC-0.100000        0    -0.83536   1.87846   9.87463  L
H-HC-0.100000        0    -1.57336   3.00053   11.03965  L
H-HC-0.100000        0    -0.85233   3.61519   9.53699  L
H-HC-0.100000        0    -3.71643   1.63694   10.93582  L
H-HC-0.100000        0    -2.78845   0.56575   9.86502  L
H-HC-0.100000        0    -4.35806   1.17195   9.35098  L
N-N--0.347900        0    -5.84632   2.38271   7.18506  L
C-CT--0.263700      -1    -6.78099   1.26862   7.03693  L
C-C-0.734100         0    -6.03383  -0.05919   6.88033  L
O-O--0.589400        0    -5.19944  -0.19882   5.99442  L
C-CT--0.000700       0    -7.69497   1.49938   5.82908  L
C-CT-0.039000        0    -8.59459   0.26876   5.62641  L
C-CT-0.048600        0    -9.70948   0.52626   4.63599  L
N-N2--0.529500       0    -9.20475   0.72269   3.27026  L
C-CA-0.807600        0    -9.18961   1.82857   2.55918  L
N-N2--0.862700       0    -9.79512   2.92874   2.88989  L
N-N2--0.862700       0    -8.53558   1.82197   1.44531  L
H-H-0.274700         0    -5.22207   2.59067   6.40878  L
H-H1-0.156000        0    -7.4091    1.19512   7.92729  L
H-HC-0.032700        0    -7.09477   1.66382   4.93185  L
H-HC-0.032700        0    -8.30603   2.38254   6.0091   L
H-HC-0.028500        0    -9.04935  -0.01033   6.57792  L
H-HC-0.028500        0    -8.00252  -0.56351   5.25463  L
H-H1-0.068700        0    -10.24006   1.40384   4.98827  L
H-H1-0.068700        0    -10.38372  -0.32965   4.64984  L
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 H-H-0.345600         0    -8.77337  -0.05761   2.78355  L
 H-H-0.447800         0    -9.74515   3.67614   2.20172  L
 H-H-0.447800         0    -10.57541   2.87402   3.55086  L
 H-H-0.447800         0    -8.54855   2.68334   0.89825  L
 H-H-0.447800         0    -8.16133   0.93381   1.11899  L
 N-N--0.415700        0    -6.3796   -1.06207   7.6816   L
 C-CT--0.059700       -1   -5.97757  -2.4559    7.43488  L
 C-C-0.597300         0    -6.89453  -3.06332   6.3634   L
 O-O--0.567900        0    -8.1026   -2.84194   6.386    L
 C-CT-0.130300        0    -6.13394  -3.26601   8.74424  L
 C-CT--0.043000       0    -5.37472  -2.66933   9.95345  L
 C-CT--0.320400       0    -5.72765  -4.73407   8.53857  L
 C-CT--0.066000       0    -3.8924   -2.35606   9.71444  L
 H-H-0.271900         0    -7.14728  -0.89781   8.32133  L
 H-H1-0.086900        0    -4.94324  -2.49538   7.09373  L
 H-HC-0.018700        0    -7.19205  -3.26581   9.01383  L
 H-HC-0.023600        0    -5.45149  -3.36063   10.79363  L
 H-HC-0.023600        0    -5.86903  -1.74623   10.25952  L
 H-HC-0.088200        0    -6.41224  -5.22393   7.84543  L
 H-HC-0.088200        0    -5.79279  -5.27007   9.48384  L
 H-HC-0.088200        0    -4.7139   -4.78654   8.14343  L
 H-HC-0.018600        0    -3.42676  -2.07222   10.65843  L
 H-HC-0.018600        0    -3.80743  -1.52146   9.02329  L
 H-HC-0.018600        0    -3.37157  -3.22046   9.30589  L
 N-N--0.516300        0    -6.36165  -3.87114   5.44981  L
 C-CT-0.039700        -1   -7.153    -4.4118    4.33505  L
 C-C-0.536600         0    -7.26015  -5.94254   4.29194  L
 O-O--0.581900        0    -6.60631  -6.59244   3.47872  L
 C-CT-0.056000        0    -6.62304  -3.81507   3.00448  L    H-HC
485   0.        0.
 C-CT-0.013600        0    -6.82585  -2.28975   2.90998  H
 C-C-0.805400         0    -7.08558  -1.68936   1.53054  H
 O-O2--0.818800       0    -6.26224  -1.94054   0.51922  H
 O-O2--0.818800       0    -8.00546  -0.91383   1.36177  H
 H-H-0.293600         0    -5.35025  -3.93338   5.42747  L
 H-H1-0.110500        0    -8.1861   -4.0735    4.4113   L
 H-HC--0.017300       0    -7.16197  -4.27886   2.18574  L
 H-HC--0.017300       0    -5.56373  -4.04806   2.88271  L
 H-HC--0.042500       0    -5.95353  -1.8057    3.36085  H
 H-HC--0.042500       0    -7.70352  -2.01121   3.49074  H
 N-N--0.516300        0    -8.10211  -6.53952   5.14257  L
 C-CT-0.038100        -1   -8.36204  -7.98475   5.19027  L
 C-C-0.536600         0    -9.50412  -8.43276   4.25782  L
 O-O--0.581900        0    -10.68935  -8.2376    4.50568  L
 C-CT--0.030300       0    -8.59241  -8.46575   6.63528  L
 C-C-0.799400         0    -9.81303  -7.8594    7.32581  L
 O-O2--0.801400       0    -9.98965  -6.62417   7.24272  L
 O-O2--0.801400       0    -10.54123  -8.60797   8.01595  L
 H-H-0.293600         0    -8.65147  -5.99488   5.80126  L
 H-H1-0.088000        0    -7.45851  -8.49453   4.85457  L
 H-HC--0.012200       0    -7.71528  -8.23383   7.23755  L
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H-HC--0.012200       0    -8.69486  -9.55238   6.61878  L
N-N--0.415700        0    -9.12091  -9.07904   3.16151  L
C-CT--0.038900       -1   -9.98963  -9.61542   2.09607  L
C-C-0.597300         0    -9.4471   -10.92622   1.50812  L
O-O--0.567900        0    -10.07568  -11.52733   0.63558  L
C-CT-0.365400        0    -10.12845  -8.58139   0.95729  L
O-OH--0.676100       0    -8.86205  -8.15841   0.49035  L
C-CT--0.243800       0    -10.87511  -7.31332   1.36955  L
H-H-0.271900         0    -8.12444  -9.06746   2.98426  L
H-H1-0.100700        0    -10.97977  -9.82151   2.50132  L
H-H1-0.004300        0    -10.67687  -9.03414   0.13042  L
H-HC-0.064200        0    -10.2896  -6.75488   2.09995  L
H-HC-0.064200        0    -11.83634  -7.57338   1.81174  L
H-HC-0.064200        0    -11.03387  -6.68029   0.49709  L
H-HO-0.410200        0    -8.67401  -8.69478  -0.32295  L
N-N--0.516300        0    -8.28532  -11.38571   1.98393  L
C-CT-0.038100        -1   -7.47854  -12.46611   1.41686  L
C-C-0.536600         0    -7.1232   -13.5233   2.49556  L
N-N--0.415700        0    -8.15018  -14.15885   3.0786   L
C-CT--0.149000       -1   -8.02605  -15.17201   4.13471  L
O-O--0.581900        0    -5.96046  -13.76698   2.81852  L
C-CT--0.030300       0    -6.25335  -11.828    0.73365  L
C-C-0.799400         0    -5.64002  -12.73769  -0.32198  L
O-O2--0.801400       0    -4.40162  -12.92599  -0.32172  L
O-O2--0.801400       0    -6.41358  -13.16842  -1.20857  L
H-H-0.293600         0    -7.81403  -10.8032   2.66003  L
H-H-0.271900         0    -9.07286  -13.8803   2.78117  L
H-H1-0.088000        0    -8.0632   -12.98009   0.65486  L
H-HC--0.012200       0    -5.50755  -11.54769   1.47986  L
H-HC--0.012200       0    -6.56851  -10.91802   0.21978  L
H-H1-0.097600        0    -7.46622  -16.03076   3.75904  L
H-H1-0.097600        0    -9.01359  -15.50335   4.45922  L
H-H1-0.097600        0    -7.49124  -14.75175   4.98865  L
N-N--0.347900        0    -3.44948  -14.53045   1.88316  L
C-CT--0.263700       -1   -2.27739  -14.90681   2.69413  L
C-C-0.734100         0    -2.24289  -14.1019   4.01944  L
N-N--0.415700        0    -3.41186  -13.91446   4.65538  L
C-CT--0.149000       -1   -3.61028  -13.24312   5.94916  L
O-O--0.589400        0    -1.18278  -13.66185   4.45895  L
C-CT--0.000700       0    -1.00222  -14.72745   1.84318  L
C-CT-0.039000        0    -1.02584  -15.54061   0.52551  L
C-CT-0.048600        0    -0.72861  -14.69598  -0.72177  L
N-N2--0.529500       0    -1.6702   -13.56701  -0.88289  L
C-CA-0.807600        0    -1.3704   -12.33459  -1.23998  L
N-N2--0.862700       0    -0.18169  -11.98306  -1.61801  L
N-N2--0.862700       0    -2.28772  -11.4216  -1.21766  L
H-H-0.271900         0    -4.23747  -14.21849   4.15738  L
H-H-0.274700         0    -3.35932  -13.94905   1.05265  L
H-H-0.274700         0    -4.39213  -14.59621   2.26193  L
H-H1-0.156000        0    -2.3537   -15.9581   2.97282  L
H-HC-0.032700        0    -0.13934  -15.05162   2.4277   L
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H-HC-0.032700        0    -0.86638  -13.66495   1.63397  L
H-HC-0.028500        0    -1.98826  -16.03333   0.38603  L
H-HC-0.028500        0    -0.27417  -16.32825   0.59126  L
H-H1-0.068700        0    -0.78657  -15.33651  -1.60443  L
H-H1-0.068700        0     0.29603  -14.32775  -0.64412  L
H-H-0.345600         0    -2.66679  -13.70682  -0.74478  L
H-H-0.447800         0    -0.0568   -11.07296  -2.0419   L
H-H-0.447800         0     0.38884  -12.74415  -1.96871  L
H-H-0.447800         0    -2.07753  -10.51889  -1.62634  L
H-H-0.447800         0    -3.21349  -11.73167  -0.9304   L
H-H1-0.097600        0    -3.87982  -12.19866   5.78195  L
H-H1-0.097600        0    -2.69013  -13.27443   6.53632  L
H-H1-0.097600        0    -4.40752  -13.73476   6.50781  L
N-N--0.415700        0    -0.26393  -9.01007   11.45882  L
C-CT--0.149000      -1    -0.12309  -8.11476   10.30414  L
C-C-0.597300         0    -1.05529  -6.91051   10.48308  L
N-N--0.415700        0    -2.36794  -7.14897   10.43629  L
C-CT--0.149000       0    -3.39593  -6.17408   10.78369  L
O-O--0.567900        0    -0.58656  -5.8091    10.76979  L
C-CT--0.015200       0    -0.2847   -8.9279    9.01314  L
C-CA--0.001100       0     0.45862  -10.25936   9.00537  L
C-CA--0.190600       0     1.75398  -10.36964   9.55854  L
C-CA--0.190600       0    -0.16398  -11.40429   8.46872  L
C-CA--0.234100       0     2.40614  -11.61667   9.60755  L
C-CA--0.234100       0     0.50104  -12.6447   8.48197  L
C-C-0.322600         0     1.78092  -12.75821   9.06115  L
O-OH--0.557900       0     2.40955  -13.96059   9.07404  L
H-H-0.271900         0    -2.63887  -8.10208   10.24592  L
H-H-0.271900         0    -0.06402  -9.9974    11.33788  L
H-H-0.271900         0    -0.47536  -8.64055   12.37745  L
H-H1-0.087600        0     0.89334  -7.72061   10.31433  L
H-HC-0.029500        0     0.07596  -8.3263    8.17858  L
H-HC-0.029500        0    -1.34451  -9.13318   8.86658  L
H-HA-0.169900        0     2.25714  -9.50133   9.96194  L
H-HA-0.169900        0    -1.15819  -11.34854   8.04503  L
H-HA-0.165600        0     3.39159  -11.69335   10.04307  L
H-HA-0.165600        0     0.03863  -13.52721   8.06179  L
H-HO-0.399200        0     3.23964  -13.94772   9.55127  L
H-H1-0.097600        0    -3.35493  -5.33738   10.08724  L
H-H1-0.097600        0    -3.22329  -5.7961    11.79337  L
H-H1-0.097600        0    -4.3821   -6.63851   10.74142  L
N-N--0.415700        0     1.83192  -4.31535   11.8946  L
C-CT--0.059700      -1     2.22614  -3.07605   11.2064  L
C-C-0.597300         0     2.25714  -1.87078   12.16231  L
N-N--0.415700        0     1.23778  -1.71939   13.01584  L
C-CT--0.149000       0     1.12294  -0.63269   13.98869  L
O-O--0.567900        0     3.201    -1.08307   12.11405  L
C-CT-0.130300        0     1.30416  -2.86423   9.97022  L
C-CT--0.043000       0     1.77504  -3.62155   8.7029   L
C-CT--0.320400       0     1.16874  -1.38459   9.56061  L
C-CT--0.066000       0     2.1458   -5.1019    8.8487   L
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H-H-0.271900          0      0.51173  -2.41903   12.98436  L
H-H-0.271900          0      1.04683  -4.85709   11.5315   L
H-H-0.271900          0      2.34689  -4.64163   12.7022   L
H-H1-0.086900         0      3.24725  -3.19123   10.84618  L
H-HC-0.018700         0      0.30187  -3.21659   10.22184  L
H-HC-0.023600         0      2.63909  -3.11354   8.28473   L
H-HC-0.023600         0      0.98013  -3.55811   7.96017   L
H-HC-0.088200         0      2.15501  -0.94966   9.39506   L
H-HC-0.088200         0      0.64442  -0.81922   10.33128  L
H-HC-0.088200         0      0.59135  -1.30471   8.64026   L
H-HC-0.018600         0      2.47208  -5.48064   7.883     L
H-HC-0.018600         0      1.28094  -5.6767    9.16033   L
H-HC-0.018600         0      2.96006  -5.2326    9.56      L
H-H1-0.097600         0      0.97095   0.31859   13.47574  L
H-H1-0.097600         0      2.03809  -0.5585    14.58082  L
H-H1-0.097600         0      0.28296  -0.81159   14.66172  L
N-N--0.415700         0      5.09533   0.98301   12.79118  L
C-CT--0.051800       -1      4.50921   2.32764   12.78384  L
C-C-0.597300          0      3.91074   2.66396   14.15767  L
N-N--0.415700         0      4.53049   3.59502   14.89211  L
C-CT--0.149000        0      4.08056   4.02318   16.21643  L
O-O--0.567900         0      2.89074   2.09334   14.53281  L
C-CT-0.110200         0      3.40091   2.42516   11.72026  L
C-CT-0.353100         0      3.87888   2.16955   10.28054  L
C-CT--0.412100        0      2.69136   2.22879   9.32303   L
C-CT--0.412100        0      4.9356    3.17738   9.81642   L
H-H-0.271900          0      5.36771   4.01933   14.52451  L
H-H-0.271900          0      4.47504   0.18799   12.63095  L
H-H-0.271900          0      5.99369   0.81949   13.22663  L
H-H1-0.092200         0      5.2852    3.05937   12.562    L
H-HC-0.045700         0      2.95484   3.41968   11.76999  L
H-HC-0.045700         0      2.62214   1.69754   11.95572  L
H-HC--0.036100        0      4.29844   1.17074   10.21655  L
H-HC-0.100000         0      2.2374    3.2193    9.34316   L
H-HC-0.100000         0      1.94754   1.49065   9.62014   L
H-HC-0.100000         0      3.02675   1.99845   8.31113   L
H-HC-0.100000         0      5.18599   2.9906    8.77523   L
H-HC-0.100000         0      5.84843   3.06654   10.39998  L
H-HC-0.100000         0      4.55964   4.19638   9.91521   L
H-H1-0.097600         0      4.74717   4.7897    16.61569  L
H-H1-0.097600         0      4.06998   3.17053   16.899    L
H-H1-0.097600         0      3.06838   4.42821   16.15343  L
N-N--0.415700         0    -12.41682   0.37641   9.35423   L
C-CT--0.001400       -1    -11.2793   -0.03074   10.18803  L
C-C-0.597300          0    -10.44175  -1.12996   9.52913   L
O-O--0.567900         0    -9.23923   -0.97014   9.30897   L
C-CT--0.015200        0    -11.77343  -0.43222   11.58607  L
C-CA--0.001100        0    -12.50294   0.68458   12.30947  L
C-CA--0.190600        0    -11.77531   1.77778   12.81936  L
C-CA--0.190600        0    -13.90571   0.64776   12.4471   L
C-CA--0.234100        0    -12.44806   2.83307   13.46411  L
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C-CA--0.234100       0    -14.5808   1.70132   13.09497  L
C-C-0.322600         0    -13.85041   2.79747   13.60455  L
O-OH--0.557900       0    -14.48811   3.82212   14.22668  L
H-H-0.271900         0    -13.17043   0.90096   9.78169  L
H-H-0.271900         0    -12.3916   0.25692   8.34648  L
H-H1-0.087600        0    -10.6215   0.83209   10.30355  L
H-HC-0.029500        0    -10.91337  -0.72782   12.18901  L
H-HC-0.029500        0    -12.43162  -1.29862   11.50481  L
H-HA-0.169900        0    -10.69873   1.81163   12.72081  L
H-HA-0.169900        0    -14.47152  -0.18953   12.06156  L
H-HA-0.165600        0    -11.90703   3.67702   13.8656  L
H-HA-0.165600        0    -15.65465   1.67197   13.20352  L
H-HO-0.399200        0    -15.42146   3.64679   14.35502  L
N-N--0.347900        0    -11.11241  -2.23881   9.21512  L
C-CT--0.263700      -1    -10.59337  -3.43197   8.54813  L
C-C-0.734100         0    -11.69219  -3.97058   7.62923  L
O-O--0.589400        0    -12.85378  -3.99481   8.0355   L
C-CT--0.000700       0    -10.08386  -4.41359   9.62657  L
C-CT-0.039000        0    -11.16782  -5.0828    10.49529  L
C-CT-0.048600        0    -11.61234  -6.42653   9.90884  L
N-N2--0.529500       0    -12.72907  -7.02993   10.65608  L
C-CA-0.807600        0    -13.14753  -8.27675   10.53111  L
N-N2--0.862700       0    -12.58872  -9.13364   9.72731  L
N-N2--0.862700       0    -14.16204  -8.69895   11.23275  L
H-H-0.274700         0    -12.10953  -2.23224   9.38717  L
H-H1-0.156000        0    -9.75127  -3.1424    7.93072  L
H-HC-0.032700        0    -9.42447  -3.85463   10.2928  L
H-HC-0.032700        0    -9.45915  -5.1763    9.16535  L
H-HC-0.028500        0    -12.02545  -4.41924   10.60903  L
H-HC-0.028500        0    -10.75027  -5.27084   11.48519  L
H-H1-0.068700        0    -10.75266  -7.09763   9.93185  L
H-H1-0.068700        0    -11.9181  -6.29332   8.87181  L
H-H-0.345600         0    -13.25011  -6.42375   11.26229  L
H-H-0.447800         0    -12.88563  -10.0803   9.63246  L
H-H-0.447800         0    -11.8091  -8.81401   9.13294  L
H-H-0.447800         0    -14.46673  -9.64757   11.12812  L
H-H-0.447800         0    -14.63374  -8.07888   11.86416  L
N-N--0.415700        0    -11.34796  -4.28467   6.38624  L
C-CT--0.003100      -1    -12.28993  -4.55059   5.29217  L
C-C-0.597300         0    -13.15857  -5.8212    5.43853  L
N-N--0.415700        0    -12.7796  -6.78393   6.28762  L
C-CT--0.149000      -1    -13.54809  -7.99644   6.57463  L
O-O--0.567900        0    -14.18917  -5.92086   4.76845  L
C-CT--0.003600       0    -11.53392  -4.5632    3.95264  L
C-CT--0.064500       0    -11.03442  -3.1527    3.60981  L
C-C-0.695100         0    -10.39095  -3.0457    2.23346  L
O-O--0.608600        0    -9.65727  -3.91357   1.77208  L
N-N--0.940700        0    -10.60651  -1.94437   1.55427  L
H-H-0.271900         0    -10.35822  -4.32087   6.20259  L
H-H-0.271900         0    -11.85278  -6.68413   6.69869  L
H-H1-0.085000        0    -13.00155  -3.72336   5.26054  L
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H-HC-0.017100        0    -12.20946  -4.89037   3.1608   L
H-HC-0.017100        0    -10.69388  -5.2573    4.0079   L
H-HC-0.035200        0    -10.29935  -2.83394   4.34822  L
H-HC-0.035200        0    -11.87945  -2.46429   3.65403  L
H-H-0.425100         0    -9.83642  -1.70622   0.93797  L
H-H-0.425100         0    -11.19936  -1.22803   1.9482   L
H-H1-0.097600        0    -12.85986  -8.80368   6.82828  L
H-H1-0.097600        0    -14.1235  -8.29023   5.69565  L
H-H1-0.097600        0    -14.22749  -7.81166   7.40632  L
N-N--0.347900        0    -14.89396  -14.74908  -4.3806   L
C-CT--0.240000       -1   -14.84359  -13.27916  -4.42925  L
C-C-0.734100         0    -15.5853  -12.7303  -5.67648  L
N-N-0.415700         0    -16.00825  -11.46374  -5.76419  L
C-CT-0.149000        0    -15.98329  -10.4136  -4.75542  L
O-O--0.589400        0    -15.77281  -13.47655  -6.62583  L
C-CT--0.009400       0    -13.35353  -12.82916  -4.46375  L
C-CT-0.018700        0    -12.49314  -13.15741  -3.21909  L
C-CT--0.047900       0    -11.10189  -12.47664  -3.26828  L
C-CT--0.014300       0    -10.14449  -12.99915  -2.1768   L
N-N3--0.385400       0    -8.84486  -12.27375  -2.14648  L
H-H-0.274700         0    -16.42749  -11.27114  -6.66133  L
H-H-0.271900         0    -14.65691  -15.26458  -3.53874  L
H-H-0.271900         0    -15.11124  -15.27159  -5.22783  L
H-H1-0.142600        0    -15.3127  -12.8996  -3.51957  L
H-HC-0.036200        0    -13.3239  -11.75253  -4.60795  L
H-HC-0.036200        0    -12.87288  -13.27774  -5.33635  L
H-HC-0.010300        0    -12.3592  -14.23843  -3.15994  L
H-HC-0.010300        0    -13.01487  -12.8221  -2.32154  L
H-HC-0.062100        0    -11.22988  -11.3994  -3.145    L
H-HC-0.062100        0    -10.64719  -12.66206  -4.24322  L
H-HP-0.113500        0    -9.95845  -14.06183  -2.3555   L
H-HP-0.113500        0    -10.62642  -12.90151  -1.199    L
H-H-0.340000         0    -8.4051   -12.17207  -3.05078  L
H-H-0.340000         0    -8.13465  -12.75173  -1.58633  L
H-H-0.340000         0    -8.91999  -11.33378  -1.75114  L
H-H1-0.097600        0    -15.63981  -10.78947  -3.79261  L
H-H1-0.097600        0    -16.98679  -10.00482  -4.62625  L
H-H1-0.097600        0    -15.32244  -9.60955  -5.08014  L
N-N--0.254800        0    -15.82932  -8.99973  -1.64116  L
C-CT--0.026600       -1   -14.74344  -8.05132  -1.85323  L
C-C-0.589600         0    -13.63891  -8.56298  -2.7824   L
O-O--0.574800        0    -13.48515  -9.76107  -3.03048  L
C-CT--0.007000       0    -14.21456  -7.74082  -0.44636  L
C-CT-0.018900        0    -15.4737  -7.8496    0.41468  L
C-CT-0.019200        0    -16.20215  -9.02923  -0.23567  L
H-H1-0.064100        0    -15.17081  -7.14087  -2.27611  L
H-HC-0.025300        0    -13.77185  -6.74707  -0.38505  L
H-HC-0.025300        0    -13.49385  -8.50121  -0.13814  L
H-HC-0.021300        0    -16.07201  -6.94349   0.3048   L
H-HC-0.215300        0    -15.24405  -8.0262    1.46976  L
H-H1-0.039100        0    -15.86192  -9.96612   0.20793  L
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H-H1-0.039100        0    -17.2814  -8.92692  -0.11358  L
N-N--0.415700        0    -12.90578  -7.61935  -3.3601   L
C-CT--0.038900       -1   -11.69848  -7.73137  -4.20146  L
C-C-0.597300         0    -11.11556  -6.32313  -4.18     L
O-O--0.567900        0    -11.88047  -5.36395  -4.29841  L
C-CT-0.365400        0    -12.04714  -8.15552  -5.64176  L
O-OH--0.676100       0    -12.83824  -9.32975  -5.60713  L
C-CT--0.243800       0    -10.80158  -8.48249  -6.45884  L
H-H-0.271900         0    -13.14723  -6.66145  -3.13622  L
H-H1-0.100700        0    -10.98726  -8.43303  -3.76107  L
H-H1-0.004300        0    -12.61045  -7.36281  -6.13596  L
H-HC-0.064200        0    -10.16417  -7.60244  -6.5432   L
H-HC-0.064200        0    -11.0951  -8.7994   -7.4599   L
H-HC-0.064200        0    -10.2417  -9.28557  -5.97897  L
H-HO-0.410200        0    -12.78344  -9.62474  -4.6831   L
N-N--0.415700        0    -9.81854  -6.17858  -3.94119  L
C-CT--0.001400       -1   -9.14715  -4.91181  -3.63161  L
C-C-0.597300         0    -9.55589  -3.75356  -4.55255  L
O-O--0.567900        0    -10.05518  -2.75696  -4.04444  L
C-CT--0.015200       0    -7.65564  -5.19172  -3.63405  L
C-CA--0.001100       0    -6.79961  -3.9536   -3.76441  L
C-CA--0.190600       0    -6.17152  -3.68334  -4.99387  L
C-CA--0.190600       0    -6.73018  -3.02241  -2.71075  L
C-CA--0.234100       0    -5.55654  -2.44069  -5.20146  L
C-CA--0.234100       0    -6.11125  -1.77684  -2.91908  L
C-C-0.322600         0    -5.57479  -1.4658   -4.18497  L
O-OH--0.557900       0    -5.13011  -0.21536  -4.46129  L
H-H-0.271900         0    -9.25247  -7.02566  -3.87175  L
H-H1-0.087600        0    -9.41558  -4.61208  -2.6176   L
H-HC-0.029500        0    -7.40692  -5.87761  -4.44588  L
H-HC-0.029500        0    -7.47177  -5.69476  -2.69141  L
H-HA-0.169900        0    -6.21046  -4.39129  -5.81209  L
H-HA-0.169900        0    -7.19922  -3.22602  -1.75432  L
H-HA-0.165600        0    -5.11507  -2.20626  -6.15859  L
H-HA-0.165600        0    -6.11126  -1.04262  -2.12523  L
H-HO-0.399200        0    -4.92304   0.28757  -3.64731  L
N-N--0.415700        0    -9.46341  -3.91548  -5.8811   L
C-CT-0.014300        -1   -9.87462  -2.93342  -6.90722  L
C-C-0.597300         0    -11.34124  -2.45947  -6.86748  L
O-O--0.567900        0    -11.72324  -1.60658  -7.65864  L
C-CT--0.204100       0    -9.45355  -3.44731  -8.29865  L
C-C-0.713000         0    -8.14001  -2.82891  -8.74109  L
O-O--0.593100        0    -7.16009  -2.78058  -8.01836  L
N-N--0.919100        0    -8.08259  -2.27777  -9.92269  L
H-H-0.271900         0    -8.99655  -4.75249  -6.1906   L
H-H1-0.104800        0    -9.30726  -2.02266  -6.70606  L
H-HC-0.079700        0    -10.21747  -3.18389  -9.03184  L
H-HC-0.079700        0    -9.3513   -4.53116  -8.30157  L
H-H-0.419600         0    -7.23084  -1.80159  -10.14687  L
H-H-0.419600         0    -8.95794  -2.08875  -10.40529  L
N-N--0.415700        0    -12.13651  -2.95812  -5.9242   L
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C-CT--0.002400       -1   -13.44539  -2.43632  -5.55327  L
C-C-0.597300         0    -13.53027  -2.06012  -4.07283  L
O-O--0.567900        0    -13.99624  -0.97641  -3.73557  L
C-CT--0.034300       0    -14.51904  -3.4637   -5.93721  L
C-CA-0.011800        0    -15.92936  -3.0288   -5.58771  L
C-CA--0.125600       0    -16.62225  -2.14691  -6.43795  L
C-CA--0.125600       0    -16.53807  -3.47451  -4.3975   L
C-CA--0.170400       0    -17.91933  -1.71898  -6.10427  L
C-CA--0.170400       0    -17.83602  -3.04661  -4.06512  L
C-CA--0.107200       0    -18.5265  -2.16903  -4.9192   L
H-H-0.271900         0    -11.71538  -3.64391  -5.31412  L
H-H1-0.097800        0    -13.64531  -1.52205  -6.11686  L
H-HC-0.029500        0    -14.30608  -4.41073  -5.43966  L
H-HC-0.029500        0    -14.46638  -3.63838  -7.01311  L
H-HA-0.133000        0    -16.15695  -1.78301  -7.34397  L
H-HA-0.133000        0    -16.00598  -4.12871  -3.72476  L
H-HA-0.143000        0    -18.44612  -1.03299  -6.75406  L
H-HA-0.143000        0    -18.30255  -3.37265  -3.14639  L
H-HA-0.129700        0    -19.51972  -1.82723  -4.66076  L
N-N--0.415700        0    -13.06728  -2.94396  -3.18571  L
C-CT-0.033700        -1   -13.02239  -2.71074  -1.74472  L
C-C-0.597300         0    -12.35242  -1.37343  -1.38505  L
O-O--0.567900        0    -12.93116  -0.56681  -0.66016  L
C-CT--0.182500       0    -12.32948  -3.90507  -1.0756   L
H-H-0.271900         0    -12.64363  -3.7851   -3.55212  L
H-H1-0.082300        0    -14.04762  -2.65715  -1.37448  L
H-HC-0.060300        0    -12.83079  -4.82956  -1.35455  L
H-HC-0.060300        0    -12.37347  -3.78771   0.00836  L
H-HC-0.060300        0    -11.28331  -3.95297  -1.37889  L
N-N--0.415700        0    -11.16367  -1.12416  -1.94444  L
C-CT--0.087500       -1   -10.43227   0.14076  -1.81307  L
C-C-0.597300         0    -11.25123   1.34608  -2.25561  L
O-O--0.567900        0    -11.17423   2.38916  -1.62696  L
C-CT-0.298500        0    -9.07197   0.06818  -2.53857  L
C-CT--0.319200       0    -9.13887   0.28079  -4.05638  L
C-CT--0.319200       0    -8.06948   1.07511  -1.97114  L
H-H-0.271900         0    -10.77224  -1.82876  -2.56002  L
H-H1-0.096900        0    -10.22601   0.2818   -0.75143  L
H-HC--0.029700       0    -8.66453  -0.92566  -2.36086  L
H-HC-0.079100        0    -8.19073  -0.02608  -4.49222  L
H-HC-0.079100        0    -9.31487   1.33235  -4.28873  L
H-HC-0.079100        0    -9.93285  -0.31798  -4.49436  L
H-HC-0.079100        0    -7.82695   0.80338  -0.94595  L
H-HC-0.079100        0    -8.48949   2.08023  -1.99797  L
H-HC-0.079100        0    -7.15171   1.05983  -2.55658  L
N-N--0.415700        0    -12.03809   1.20832  -3.32383  L
C-CT--0.087500       -1   -12.83082   2.29073  -3.9136   L
C-C-0.597300         0    -13.95968   2.73128  -2.9911   L
O-O--0.567900        0    -14.11875   3.92186  -2.7352   L
C-CT-0.298500        0    -13.37061   1.92106  -5.31281  L
C-CT--0.319200       0    -13.98748   3.13999  -6.00908  L
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| | | | | | |
|---|---|---|---|---|---|
| C-CT--0.319200 | 0 | -12.25606 | 1.38606 | -6.22251 | L |
| H-H-0.271900 | 0 | -12.11191 | 0.28816 | -3.72795 | L |
| H-H1-0.096900 | 0 | -12.17404 | 3.15351 | -4.03332 | L |
| H-HC--0.029700 | 0 | -14.13777 | 1.15327 | -5.22159 | L |
| H-HC-0.079100 | 0 | -14.33275 | 2.86254 | -7.00604 | L |
| H-HC-0.079100 | 0 | -13.24604 | 3.93414 | -6.10414 | L |
| H-HC-0.079100 | 0 | -14.84074 | 3.51159 | -5.442 | L |
| H-HC-0.079100 | 0 | -11.86135 | 0.45007 | -5.83455 | L |
| H-HC-0.079100 | 0 | -11.45449 | 2.12041 | -6.29361 | L |
| H-HC-0.079100 | 0 | -12.65453 | 1.19422 | -7.21966 | L |
| N-N--0.415700 | 0 | -14.73196 | 1.77267 | -2.47508 | L |
| C-CT--0.087500 | -1 | -15.76402 | 2.02611 | -1.45899 | L |
| C-C-0.597300 | 0 | -15.16258 | 2.71891 | -0.24213 | L |
| O-O--0.567900 | 0 | -15.62749 | 3.77597 | 0.1732 | L |
| C-CT-0.298500 | 0 | -16.49393 | 0.72299 | -1.07008 | L |
| C-CT--0.319200 | 0 | -17.57072 | 0.96452 | -0.00353 | L |
| C-CT--0.319200 | 0 | -17.18871 | 0.09101 | -2.28523 | L |
| H-H-0.271900 | 0 | -14.52018 | 0.8193 | -2.74801 | L |
| H-H1-0.096900 | 0 | -16.49775 | 2.71284 | -1.88107 | L |
| H-HC--0.029700 | 0 | -15.77215 | 0.00614 | -0.67688 | L |
| H-HC-0.079100 | 0 | -18.09614 | 0.03449 | 0.21261 | L |
| H-HC-0.079100 | 0 | -18.28573 | 1.70923 | -0.35493 | L |
| H-HC-0.079100 | 0 | -17.11364 | 1.31672 | 0.92151 | L |
| H-HC-0.079100 | 0 | -17.90127 | 0.7944 | -2.71689 | L |
| H-HC-0.079100 | 0 | -17.71565 | -0.8129 | -1.98228 | L |
| H-HC-0.079100 | 0 | -16.45682 | -0.18195 | -3.04464 | L |
| N-N--0.516300 | 0 | -14.13349 | 2.10962 | 0.33202 | L |
| C-CT-0.038100 | -1 | -13.52086 | 2.5042 | 1.59648 | L |
| C-C-0.536600 | 0 | -12.68309 | 3.78992 | 1.50172 | L |
| O-O--0.581900 | 0 | -12.5802 | 4.53094 | 2.47193 | L |
| C-CT--0.030300 | 0 | -12.731 | 1.2744 | 2.07161 | L |
| C-C-0.799400 | 0 | -12.57697 | 1.19487 | 3.58448 | L |
| O-O2--0.801400 | 0 | -12.20945 | 2.22054 | 4.19253 | L |
| O-O2--0.801400 | 0 | -12.71275 | 0.07421 | 4.1224 | L |
| H-H-0.293600 | 0 | -13.79134 | 1.25738 | -0.09885 | L |
| H-H1-0.088000 | 0 | -14.31738 | 2.69211 | 2.318 | L |
| H-HC--0.012200 | 0 | -11.75359 | 1.25457 | 1.58902 | L |
| H-HC--0.012200 | 0 | -13.26333 | 0.37132 | 1.76584 | L |
| N-N--0.516300 | 0 | -12.11876 | 4.12785 | 0.34122 | L |
| C-CT-0.038100 | -1 | -11.47338 | 5.42922 | 0.13463 | L |
| C-C-0.536600 | 0 | -12.44143 | 6.61296 | 0.01047 | L |
| O-O--0.581900 | 0 | -12.00429 | 7.75763 | 0.12872 | L |
| C-CT--0.030300 | 0 | -10.41452 | 5.39025 | -0.98986 | L |
| C-C-0.799400 | 0 | -9.09379 | 4.7273 | -0.55459 | L |
| O-O2--0.801400 | 0 | -8.9213 | 4.39705 | 0.64181 | L |
| O-O2--0.801400 | 0 | -8.15314 | 4.61006 | -1.37483 | L |
| H-H-0.293600 | 0 | -12.15026 | 3.47406 | -0.43508 | L |
| H-H1-0.088000 | 0 | -10.92415 | 5.66102 | 1.04728 | L |
| H-HC--0.012200 | 0 | -10.17353 | 6.41526 | -1.27595 | L |
| H-HC--0.012200 | 0 | -10.82155 | 4.89764 | -1.87269 | L |
| N-N--0.415700 | 0 | -13.74937 | 6.37009 | -0.10895 | L |

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C-CT--0.058100       -1   -14.78128   7.41308  -0.10153  L
C-C-0.597300         0    -15.74906   7.22919   1.07335  L
N-N--0.415700        0    -16.6634   6.25968   1.0021   L
C-CT--0.149000       0    -17.64391   5.94557   2.03798  L
O-O--0.567900        0    -15.63711   7.94478   2.07163  L
C-CT--0.007400       0    -15.45324   7.49315  -1.47801  L
C-CC-0.186800        0    -14.50236   8.0176   -2.52467  L
N-NB--0.543200       0    -14.06937   9.34047  -2.62066  L
C-CW--0.220700       0    -13.86451   7.2687   -3.46889  L
C-CR-0.163500        0    -13.18508   9.36086  -3.62846  L
N-NA--0.279500       0    -13.04092   8.13228  -4.15828  L
H-H-0.271900         0    -14.02524   5.39804  -0.19505  L
H-H-0.271900         0    -16.55419   5.60182   0.23727  L
H-H1-0.136000        0    -14.31258   8.38402   0.06132  L
H-HC-0.036700        0    -16.30357   8.17346  -1.42204  L
H-HC-0.036700        0    -15.81555   6.50739  -1.77433  L
H-H4-0.186200        0    -13.97357   6.20282  -3.61255  L
H-H-0.333900         0    -12.42272   7.88939  -4.92034  L
H-H5-0.143500        0    -12.65991   10.24578  -3.96212  L
H-H1-0.097600        0    -18.11213   6.86255   2.40065  L
H-H1-0.097600        0    -17.15022   5.43911   2.86867  L
H-H1-0.097600        0    -18.41269   5.2882    1.62905  L
N-N--0.415700        0    -13.95703   6.36169   3.96988  L
C-CT--0.023700       -1   -13.13887   7.04125   4.97455  L
C-C-0.597300         0    -12.95602   8.56114   4.72958  L
N-N--0.415700        0    -13.65887   9.15004   3.75631  L
C-CT--0.149000       0    -13.75605   10.58922   3.52751  L
O-O--0.567800        0    -12.22121   9.23022   5.46978  L
C-CT-0.034200        0    -11.78761   6.33261   5.16862  L
C-CT-0.001800        0    -11.94822   5.02462   5.9428   L
S-S--0.273700        0    -10.37752   4.32362   6.51541  L
C-CT--0.053600       0    -11.0108   2.85118   7.35913  L
H-H-0.271900         0    -14.24574   8.55767   3.17389  L
H-H-0.271900         0    -13.56428   5.53471   3.5193   L
H-H-0.271900         0    -14.77665   6.79491   3.55516  L
H-H1-0.088000        0    -13.67648   6.97137   5.91994  L
H-HC-0.024100        0    -11.13413   6.97015   5.76198  L
H-HC-0.024100        0    -11.30929   6.14615   4.20606  L
H-H1-0.044000        0    -12.46389   4.30531   5.31086  L
H-H1-0.044000        0    -12.56974   5.20725   6.81925  L
H-H1-0.068400        0    -11.65603   3.1526    8.18359  L
H-H1-0.068400        0    -10.17665   2.26551   7.7449   L
H-H1-0.068400        0    -11.58493   2.24646   6.6559   L
H-H1-0.097600        0    -12.76312   11.03716   3.51416  L
H-H1-0.097600        0    -14.35552   11.04818   4.31539  L
H-H1-0.097600        0    -14.24469   10.76858   2.56715  L
N-N--0.415700        0    -11.67539   10.37108   1.08593  L
C-CT--0.059700       -1   -10.30989   10.79052   1.41007  L
C-C-0.597300         0    -9.95296   11.98982   0.50872  L
N-N--0.415700        0    -10.06888   13.20452   1.0588   L
C-CT--0.149000       0    -9.79957   14.4742   0.38272  L
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O-O--0.567900        0    -9.60419   11.83362  -0.66063  L
C-CT-0.130300        0    -9.35045   9.58718   1.2206    L
C-CT--0.043000       0    -9.59255   8.47589   2.27271   L
C-CT--0.320400       0    -7.86077   9.97379   1.20052   L
C-CT--0.066000       0    -9.30579   8.85365   3.73368   L
H-H-0.271900         0    -10.3862   13.23582   2.01129  L
H-H-0.271900         0    -11.82147   9.3669    0.96556  L
H-H-0.271900         0    -12.20284   10.94723   0.44118  L
H-H1-0.086900        0    -10.26508   11.12172   2.44429  L
H-HC-0.018700        0    -9.56484   9.15344   0.24142   L
H-HC-0.023600        0    -8.9788    7.61283   2.01267   L
H-HC-0.023600        0    -10.62937   8.14818   2.22083  L
H-HC-0.088200        0    -7.27222   9.10559   0.91883   L
H-HC-0.088200        0    -7.53521   10.3569   2.16432   L
H-HC-0.088200        0    -7.66289   10.72906   0.44681  L
H-HC-0.018600        0    -9.94179   9.678     4.05083   L
H-HC-0.018600        0    -8.26236   9.12674   3.86822   L
H-HC-0.018600        0    -9.5133    7.99146   4.36234   L
H-H1-0.097600        0    -10.51722   15.23035   0.70461  L
H-H1-0.097600        0    -9.88799   14.35524  -0.70013  L
H-H1-0.097600        0    -8.7899    14.81514   0.61835  L
N-N--0.415703        0    -7.01571   13.09514  -0.88516  L
C-CT--0.058100      -1    -5.63289   12.7702  -1.22839  L
C-C-0.597300         0    -5.38909   11.25845  -1.18437  L
O-O--0.567900        0    -4.89988   10.69366  -0.20047  L
C-CT--0.007400       0    -4.70476   13.54049  -0.26965  L
C-CC-0.186800        0    -4.97007   15.02561  -0.20064  L
N-NB--0.543200       0    -5.95223   15.64029   0.58545  L
C-CW--0.220700       0    -4.29703   15.97969  -0.9039   L
C-CR-0.163500        0    -5.8468    16.95417   0.33033  L
N-NA--0.279500       0    -4.86248   17.18765  -0.55651  L
H-H-0.271900         0    -7.13789   13.79345  -0.15802  L
H-H-0.271900         0    -7.79632   12.47653  -1.09925  L
H-H1-0.136000        0    -5.42617   13.12086  -2.23971  L
H-HC-0.036700        0    -3.66798   13.37753  -0.56258  L
H-HC-0.036700        0    -4.82785   13.14799   0.73407  L
H-H4-0.186200        0    -3.48088   15.80746  -1.59212  L
H-H-0.333900         0    -4.59151   18.0998  -0.90139  L
H-H5-0.143500        0    -6.46765   17.72179   0.77451  L
N-N--0.415700        0    -5.75907   10.5857  -2.27478  L
C-CT--0.087500      -1    -5.71264   9.12139  -2.39817  L
C-C-0.597300         0    -4.29259   8.6655   -2.74465  L
O-O--0.567900        0    -3.97908   8.25019  -3.85857  L
C-CT-0.298500        0    -6.78281   8.61922  -3.39721  L
C-CT--0.319200       0    -6.98829   7.11146  -3.24336  L
C-CT--0.319200       0    -8.15608   9.26945  -3.1573   L
H-H-0.271900         0    -6.19924   11.10531  -3.01948  L
H-H1-0.096900        0    -5.97214   8.69948  -1.43338  L
H-HC--0.029700       0    -6.47525   8.84978  -4.41559  L
H-HC-0.079100        0    -6.05784   6.57283  -3.41734  L
H-HC-0.079100        0    -7.72995   6.76474  -3.96334  L
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 H-HC-0.079100        0    -7.36417   6.89324  -2.24636  L
 H-HC-0.079100        0    -8.47437   9.1194   -2.12488  L
 H-HC-0.079100        0    -8.89536   8.8178   -3.82096  L
 H-HC-0.079100        0    -8.1271    10.33553  -3.37633  L
 N-N--0.415700        0    -3.39299   8.84615  -1.7835   L
 C-CT--0.002400       -1   -1.95412   8.71714  -1.97777  L
 C-C-0.597300         0    -1.46672   7.29938  -1.65601  L
 O-O--0.567900        0    -1.97075   6.64343  -0.73784  L
 C-CT--0.034300       0    -1.22393   9.7581   -1.1158   L
 C-CA-0.011800        0    -1.30208   11.22158  -1.53868  L
 C-CA--0.125600       0    -2.14313   11.68066  -2.57785  L
 C-CA--0.125600       0    -0.45802   12.14147  -0.88808  L
 C-CA--0.170400       0    -2.12928   13.03387  -2.96162  L
 C-CA--0.170400       0    -0.44961   13.49559  -1.26498  L
 C-CA--0.107200       0    -1.27957   13.94126  -2.30699  L
 H-H-0.271900         0    -3.72336   9.26474  -0.92312  L
 H-H1-0.097800        0    -1.70722   8.91504  -3.02181  L
 H-HC-0.029500        0    -0.16533   9.49306  -1.10792  L
 H-HC-0.029500        0    -1.58393   9.67609  -0.08982  L
 H-HA-0.133000        0    -2.77751   11.00773  -3.12901  L
 H-HA-0.133000        0     0.20906   11.80181  -0.10606  L
 H-HA-0.143000        0    -2.74024   13.3715  -3.78784  L
 H-HA-0.143000        0     0.22019   14.18676  -0.77132  L
 H-HA-0.129700        0    -1.24113   14.97546  -2.62001  L
 N-N--0.347900        0    -0.48523   6.82705  -2.43045  L
 C-CT--0.263700       -1    0.13568   5.49604  -2.35804  L
 C-C-0.734100         0     1.38938   5.39576  -3.22657  L
 O-O--0.589400        0     1.8846    6.42035  -3.68287  L
 C-CT--0.000700       0    -0.90352   4.43211  -2.76985  L
 C-CT-0.039000        0    -1.50485   4.60921  -4.17152  L    H-H1
1046  0.        0.
 C-CT-0.048600        0    -2.63822   3.60034  -4.33004  H
 N-N2--0.529500       0    -3.29585   3.76224  -5.61931  H
 C-CA-0.807600        0    -4.5417    3.34773  -5.82161  H
 N-N2--0.862700       0    -5.24153   2.80682  -4.83227  H
 N-N2--0.862700       0    -5.09448   3.46067  -7.04392  H
 H-H-0.274700         0    -0.17876   7.41362  -3.20457  L
 H-H1-0.156000        0     0.44356   5.29534  -1.33187  L
 H-HC-0.032700        0    -1.70907   4.45558  -2.0452   L
 H-HC-0.032700        0    -0.46416   3.43745  -2.70882  L
 H-HC-0.028500        0    -0.74216   4.43708  -4.93166  L
 H-HC-0.028500        0    -1.91137   5.61468  -4.28753  L
 H-H1-0.068700        0    -3.37262   3.78322  -3.54153  H
 H-H1-0.068700        0    -2.25359   2.58484  -4.20076  H
 H-H-0.345600         0    -2.74761   3.94436  -6.4472   H
 H-H-0.447800         0    -6.19471   2.53583  -5.08568  H
 H-H-0.447800         0    -4.81907   2.34578  -4.01241  H
 H-H-0.447800         0    -6.06657   3.16254  -7.10629  H
 H-H-0.447800         0    -4.80028   4.16728  -7.70824  H
 N-N--0.415700        0     1.89246   4.18427  -3.46447  L
 C-CT--0.025200       -1    3.038     3.91184  -4.33023  L
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 C-C-0.597300          0     2.6969    3.75412  -5.81186  L
 O-O--0.567900         0     1.55905   3.51357  -6.2219   L
 H-H-0.271900          0     1.42673   3.37735  -3.06346  L
 H-H1-0.069800         0     3.50322   2.98221  -4.0025   L
 H-H1-0.069800         0     3.76669   4.71112  -4.21169  L
 N-N--0.516300         0     3.74575   3.86959  -6.61586  L
 C-CT-0.039700         0     3.82725   3.60532  -8.05459  L
 C-C-0.536600          0     3.30878   2.20905  -8.43793  L
 O-O--0.581900         0     2.68368   2.0476   -9.48564  L
 C-CT-0.056000         0     5.29223   3.83305  -8.4353   L
 C-CT-0.013600         0     5.66424   3.61895  -9.90248  L
 C-C-0.805400          0     7.09574   4.12082  -10.13808  L
 O-O2--0.818800        0     8.03218   3.65273  -9.44928  L
 O-O2--0.818800        0     7.3005    5.02601  -10.97353  L
 H-H-0.293600          0     4.60514   4.17446  -6.1675   L
 H-H1-0.110500         0     3.22652   4.33672  -8.59356  L
 H-HC--0.017300        0     5.92263   3.19238  -7.81611  L
 H-HC--0.017300        0     5.51358   4.87103  -8.19203  L
 H-HC--0.042500        0     4.96238   4.1693   -10.53355  L
 H-HC--0.042500        0     5.59773   2.55634  -10.14555  L
 N-N--0.516300         0     3.47943   1.21198  -7.56135  L
 C-CT-0.038100        -1     2.93956  -0.14621  -7.71318  L
 C-C-0.536600          0     1.40125  -0.21937  -7.85147  L
 O-O--0.581900         0     0.88155  -1.25656  -8.27219  L
 C-CT--0.030300        0     3.48653  -1.06602  -6.60721  L
 C-C-0.799400          0     2.90223  -0.87978  -5.20634  L
 O-O2--0.801400        0     2.65907   0.26615  -4.7704   L
 O-O2--0.801400        0     2.774    -1.92049  -4.51499  L
 H-H-0.293600          0     3.90779   1.44172  -6.67538  L
 H-H1-0.088000         0     3.33486  -0.53009  -8.65414  L
 H-HC--0.012200        0     4.56336  -0.94547  -6.53447  L
 H-HC--0.012200        0     3.31623  -2.09545  -6.91734  L
 N-N--0.415700         0     0.68305   0.87993  -7.57977  L
 C-CT--0.058100        0    -0.76301   1.04654  -7.78972  L    H-HC
1102  0.        0.
 C-C-0.597300          0    -1.14023   2.24596  -8.69017  L
 O-O--0.567900         0    -2.31837   2.60468  -8.78317  L
 C-CT--0.007400        0    -1.44407   1.1153   -6.41655  H
 C-CC-0.186800         0    -1.47311  -0.1795   -5.66839  H
 N-NB--0.543200        0    -2.46937  -1.09804  -5.9134   H
 C-CW--0.220700        0    -0.60688  -0.6646   -4.72461  H
 C-CR-0.163500         0    -2.2102   -2.10848  -5.11489  H
 N-NA--0.279500        0    -1.08377  -1.90449  -4.38716  H
 H-H-0.271900          0     1.20357   1.65126  -7.17207  L
 H-H1-0.136000         0    -1.14919   0.16074  -8.29554  L
 H-HC-0.036700         0    -2.48801   1.41046  -6.56492  H
 H-HC-0.036700         0    -0.93948   1.89333  -5.8329   H
 H-H4-0.186200         0     0.28862  -0.25947  -4.28395  H
 H-H-0.333900          0    -0.69158  -2.51927  -3.67851  H
 H-H5-0.143500         0    -2.79535  -3.01119  -5.01952  H
 N-N--0.415700         0    -0.19108   2.83111  -9.43372  L
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C-CT--0.051800       -1   -0.4737    3.72444  -10.57505  L
C-C-0.597300         0    -1.34629   2.99148  -11.60056  L
O-O--0.567900        0    -2.47362   3.39159  -11.87968  L
C-CT--0.110200       0     0.86217   4.21018  -11.17672  L
C-CT-0.353100        0     0.73507   5.06479  -12.45273  L
C-CT--0.412100       0    -0.06245   6.34875  -12.23312  L
C-CT--0.412100       0     2.12928   5.44679  -12.94693  L
H-H-0.271900         0     0.76451   2.50432  -9.30805  L
H-H1-0.092200        0    -1.03503   4.58906  -10.22649  L
H-HC-0.045700        0     1.47368   3.34077  -11.42043  L
H-HC-0.045700        0     1.3994    4.78487  -10.42371  L
H-HC--0.036100       0     0.24675   4.47882  -13.23147  L
H-HC-0.100000        0    -1.08135   6.12014  -11.92518  L
H-HC-0.100000        0    -0.10289   6.91935  -13.16083  L
H-HC-0.100000        0     0.41894   6.95811  -11.4681  L
H-HC-0.100000        0     2.64317   6.04896  -12.19605  L
H-HC-0.100000        0     2.05166   6.02078  -13.8704  L
H-HC-0.100000        0     2.71593   4.54886  -13.1417  L
N-N--0.415700        0    -0.84087   1.8584   -12.08361  L
C-CT--0.024900       -1   -1.49468   0.88795  -12.96924  L
C-C-0.597300         0    -2.96071   0.58408  -12.6116  L
O-O--0.567900        0    -3.80608   0.53364  -13.50695  L
C-CT-0.211700        0    -0.67133  -0.40717  -12.93724  L
O-OH--0.654600       0    -0.55741  -0.85068  -11.59529  L
H-H-0.271900         0     0.06401   1.60249  -11.71189  L
H-H1-0.084300        0    -1.47835   1.28245  -13.98508  L
H-H1-0.035200        0     0.32433  -0.21003  -13.33838  L
H-H1-0.035200        0    -1.1558   -1.17376  -13.54384  L
H-HO-0.427500        0     0.14539  -1.50716  -11.51963  L
N-N--0.415700        0    -3.26479   0.34895  -11.32984  L
C-CT-0.014300        -1   -4.59676   0.00953  -10.80132  L
C-C-0.597300         0    -5.56562   1.19256  -10.77547  L
O-O--0.567900        0    -6.77065   0.96117  -10.78248  L
C-CT--0.204100       0    -4.4244   -0.6781   -9.43805  L
C-C-0.713000         0    -3.66189  -1.98874  -9.56175  L
O-O--0.593100        0    -3.72731  -2.67169  -10.57742  L
N-N--0.919100        0    -2.90538  -2.35898  -8.56008  L
H-H-0.271900         0    -2.46885   0.32381  -10.70654  L
H-H1-0.104800        0    -5.0489   -0.71618  -11.47927  L
H-HC-0.079700        0    -5.40534  -0.91473  -9.03608  L
H-HC-0.079700        0    -3.91266  -0.01138  -8.74282  L
H-H-0.419600         0    -2.44878  -3.2588   -8.63917  L
H-H-0.419600         0    -2.81839  -1.81519  -7.70711  L
N-N--0.415700        0    -5.0651    2.4315   -10.80856  L
C-CT--0.038900       -1   -5.86309   3.67038  -10.77359  L
C-C-0.597300         0    -6.99736   3.69106  -11.79701  L
O-O--0.567900        0    -8.14902   3.71748  -11.37866  L
C-CT-0.365400        0    -4.98431   4.92019  -10.70972  L
O-OH--0.676100       0    -4.18855   4.7785   -9.54726  L
C-CT--0.243800       0    -5.78699   6.20436  -10.54494  L
H-H-0.271900         0    -4.05816   2.51649  -10.88564  L
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H-H1-0.100700        0    -6.38265   3.65534  -9.81464  L
H-H1-0.004300        0    -4.35234   5.00108  -11.59187  L
H-HC-0.064200        0    -5.11211   7.04699  -10.39776  L
H-HC-0.064200        0    -6.44641   6.12126  -9.68128  L
H-HC-0.064200        0    -6.38888   6.3911   -11.43395  L
H-HO-0.410200        0    -3.51419   4.10726  -9.74017  L
N-N--0.254800        0    -6.76741   3.55307  -13.11055  L
C-CT--0.026600       -1   -7.86619   3.47101  -14.07767  L
C-C-0.589600         0    -8.57559   2.10226  -14.17952  L
O-O--0.574800        0    -9.28304   1.85148  -15.14908  L
C-CT--0.007000       0    -7.19682   3.85826  -15.40681  L
C-CT-0.018900        0    -5.77656   3.31577  -15.25448  L
C-CT-0.019200        0    -5.47865   3.60846  -13.78677  L
H-H1-0.064100        0    -8.62765   4.21785  -13.8472  L
H-HC-0.025300        0    -7.16038   4.94617  -15.48835  L
H-HC-0.025300        0    -7.69668   3.44255  -16.28233  L
H-HC-0.021300        0    -5.07451   3.82083  -15.91872  L
H-HC-0.021300        0    -5.76959   2.23845  -15.42717  L
H-H1-0.039100        0    -4.77661   2.87757  -13.39107  L
H-H1-0.039100        0    -5.06411   4.6134   -13.69675  L
N-N--0.347900        0    -8.44631   1.22124  -13.17912  L
C-CT--0.240000       -1   -9.38645   0.10688  -12.91925  L
C-C-0.734100         0    -9.88018   0.14956  -11.46215  L
O-O--0.589400        0    -10.29501  -0.86906  -10.91423  L
C-CT--0.009400       0    -8.77086  -1.268    -13.25504  L
C-CT-0.018700        0    -8.0419   -1.39869  -14.60209  L
C-CT--0.047900       0    -6.53822  -1.1454   -14.43471  L
C-CT--0.014300       0    -5.78613  -1.41054  -15.73857  L
N-N3--0.385400       0    -4.32708  -1.35534  -15.4965  L
H-H-0.274700         0    -7.81581   1.47283  -12.42504  L
H-H1-0.142600        0    -10.27326   0.23514  -13.54458  L
H-HC-0.036200        0    -9.58525  -1.99494  -13.25214  L
H-HC-0.036200        0    -8.08554  -1.55477  -12.45934  L
H-HC-0.010300        0    -8.46974  -0.71919  -15.33952  L
H-HC-0.010300        0    -8.17439  -2.42014  -14.96207  L
H-HC-0.062100        0    -6.15411  -1.81486  -13.66233  L
H-HC-0.062100        0    -6.36748  -0.11552  -14.12165  L
H-HP-0.113500        0    -6.08602  -0.66058  -16.47716  L
H-HP-0.113500        0    -6.06757  -2.39806  -16.11613  L
H-H-0.340000         0    -4.05577  -2.06441  -14.81273  L
H-H-0.340000         0    -4.08734  -0.4704   -15.05301  L
H-H-0.340000         0    -3.79524  -1.4786   -16.34479  L
N-N--0.415700        0    -9.79492   1.3316   -10.8549  L
C-CT--0.003100       -1   -10.33451   1.74084  -9.56328  L
C-C-0.597300         0    -11.2691   2.95592  -9.8082   L
N-N--0.415700        0    -10.78903   3.99254  -10.51928  L
C-CT--0.149000       -1   -11.54844   5.09572  -11.12578  L
O-O--0.567900        0    -12.43574   2.90629  -9.43232  L
C-CT--0.003600       0    -9.22804   2.03476  -8.54971  L
C-CT--0.064500       0    -8.72215   0.71077  -7.97414  L
C-C-0.695100         0    -7.54189   0.89378  -7.04351  L
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O-O--0.608600        0    -7.3271    1.93747  -6.44559  L
N-N--0.940700        0    -6.71747  -0.11177  -6.88426  L
H-H-0.271900         0    -9.38887   2.07692  -11.40039  L
H-H-0.271900         0    -9.79425   3.9798   -10.7043  L
H-H1-0.085000        0    -10.97016   0.94563  -9.16645  L
H-HC-0.017100        0    -9.63131   2.64252  -7.73876  L
H-HC-0.017100        0    -8.41168   2.57965  -9.02249  L
H-HC-0.035200        0    -8.41626   0.06789  -8.79372  L
H-HC-0.035200        0    -9.52798   0.22668  -7.42349  L
H-H-0.425100         0    -6.0221   -0.00261  -6.15366  L
H-H-0.425100         0    -6.89204  -1.0245   -7.29029  L
H-H1-0.097600        0    -11.62056   5.92098  -10.41451  L
H-H1-0.097600        0    -12.55694   4.76094  -11.37759  L
H-H1-0.097600        0    -11.04734   5.44521  -12.02907  L
N-N--0.415700        0    -5.34452   11.36772  -6.78725  L
C-CT--0.002400      -1    -4.38825   10.34892  -6.35762  L
C-C-0.597300         0    -2.93718   10.86757  -6.32481  L
O-O--0.567900        0    -2.66641   11.98437  -6.75767  L
C-CT--0.034300       0    -4.45904    9.14186  -7.31199  L
C-CA-0.011800        0    -5.71076    8.29104  -7.26971  L
C-CA--0.125600       0    -5.72922    7.10801  -6.50404  L
C-CA--0.170400       0    -6.82716    8.62909  -8.05632  L
C-CA--0.107200       0    -6.86258    6.27593  -6.51967  L
C-CA--0.170400       0    -7.9579     7.79769  -8.06711  L
C-CA--0.125600       0    -7.9747     6.61836  -7.30272  L
H-H-0.271900         0    -6.2753    11.08024  -7.06389  L
H-H-0.271900         0    -4.95495   12.24425  -7.11827  L
H-H1-0.097800        0    -4.65236   10.02452  -5.35513  L
H-HC-0.029500        0    -3.63123    8.47579  -7.07841  L
H-HC-0.029500        0    -4.30874    9.49317  -8.33399  L
H-HA-0.133000        0    -4.88001    6.83846  -5.89394  L
H-HA-0.143000        0    -6.82959    9.51097  -8.67807  L
H-HA-0.129700        0    -6.9022     5.37974  -5.91973  L
H-HA--0.170400       0    -8.80227    8.06873  -8.68157  L
H-HA--0.125600       0    -8.83566    5.96677  -7.31124  L
N-N--0.415700        0    -2.00773   10.03368  -5.84565  L
C-CT--0.023700      -1    -0.55794   10.12691  -6.07981  L
C-C-0.597300         0     0.06854    8.74473  -5.90558  L
O-O--0.567900        0    -0.4069     7.95082  -5.09046  L
C-CT-0.034200        0     0.06165   11.11686  -5.07564  L
C-CT-0.001800        0     1.5038    11.51297  -5.40617  L
S-S--0.273700        0     2.22599   12.6333  -4.17809  L
C-CT--0.053600       0     3.71388   13.16477  -5.06508  L
H-H-0.271900         0    -2.33207    9.14856  -5.4734   L
H-H1-0.088000        0    -0.38399   10.48022  -7.09792  L
H-HC-0.024100        0     0.03821   10.67809  -4.07774  L
H-HC-0.024100        0    -0.53052   12.03176  -5.0652   L
H-H1-0.044000        0     1.51283   12.00613  -6.37886  L
H-H1-0.044000        0     2.12893   10.62231  -5.45917  L
H-H1-0.068400        0     4.28988   13.84004  -4.43198  L
H-H1-0.068400        0     3.42802   13.68731  -5.97835  L
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H-H1-0.068400        0     4.3246    12.29965  -5.3189   L
N-N--0.415700        0     1.12493   8.46345  -6.66572  L
C-CT--0.058100       -1    1.68162   7.12185  -6.83335  L
C-C-0.597300         0     3.21675   7.18153  -6.75554  L
O-O--0.567900        0     3.91173   7.16658  -7.76815  L
C-CT--0.007400       0     1.18876   6.5398   -8.1697   L
C-CC-0.186800        0    -0.2467    6.85548  -8.4875   L
N-NB--0.543200       0    -0.67314   7.98209  -9.18748  L
C-CW--0.220700       0    -1.32448   6.09352  -8.16011  L
C-CR-0.163500        0    -1.99744   7.85915  -9.3135   L
N-NA--0.279500       0    -2.41553   6.73799  -8.70236  L
H-H-0.271900         0     1.40222   9.15473  -7.34678  L
H-H1-0.136000        0     1.32518   6.46598  -6.04085  L
H-HC-0.036700        0     1.31776   5.45926  -8.15145  L
H-HC-0.036700        0     1.78323   6.93973  -8.99184  L
H-H4-0.186200        0    -1.28905   5.15319  -7.63213  L
H-H-0.333900         0    -3.36769   6.38274  -8.7499   L
H-H5-0.143500        0    -2.62866   8.5539   -9.85292  L
N-N--0.415700        0     3.75991   7.33053  -5.5474   L
C-CT--0.059700       -1    5.17372   7.67081  -5.33811  L
C-C-0.597300         0     6.12389   6.50671  -5.68354  L
O-O--0.567900        0     5.82742   5.35672  -5.34549  L
C-CT-0.130300        0     5.42367   8.20998  -3.90572  L
C-CT--0.043000       0     5.1424    7.19042  -2.77687  L
C-CT--0.320400       0     4.60573   9.49814  -3.70344  L
C-CT--0.066000       0     5.49442   7.69148  -1.37023  L
H-H-0.271900         0     3.13619   7.2822   -4.74824  L
H-H1-0.086900        0     5.37081   8.49464  -6.01619  L
H-HC-0.018700        0     6.47873   8.4835   -3.84699  L
H-HC-0.023600        0     5.7188    6.28813  -2.96012  L
H-HC-0.023600        0     4.09336   6.91562  -2.7783   L
H-HC-0.088200        0     3.54238   9.27039  -3.61754  L
H-HC-0.088200        0     4.76191   10.17601  -4.54098  L
H-HC-0.088200        0     4.92766   10.00713  -2.79556  L
H-HC-0.018600        0     4.78954   8.46235  -1.05989  L
H-HC-0.018600        0     6.50539   8.09813  -1.35684  L
H-HC-0.018600        0     5.42985   6.86249  -0.66511  L
N-N--0.254800        0     7.26594   6.76761  -6.3477   L
C-CT--0.026600       -1    8.09867   5.71876  -6.93     L
C-C-0.589600         0     8.57662   4.58159  -6.037    L
O-O--0.574800        0     8.75454   4.76835  -4.83211  L
C-CT--0.007000       0     9.2939    6.44037  -7.55293  L
C-CT-0.018900        0     8.71862   7.79027  -7.95078  L
C-CT-0.019200        0     7.71672   8.07117  -6.8349   L
H-H1-0.064100        0     7.52891   5.28681  -7.74303  L
H-HC-0.025300        0     9.66752   5.90222  -8.42354  L
H-HC-0.025300        0     10.07997   6.58364  -6.80954  L
H-HC-0.021300        0     8.19057   7.69521  -8.9014   L
H-HC-0.021300        0     9.48805   8.56033  -8.01237  L
H-H1-0.039100        0     8.20399   8.61448  -6.02444  L
H-H1-0.039100        0     6.90503   8.66313  -7.2557   L
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N-N--0.415700        0     8.83396   3.42073  -6.64386  L
C-CT--0.051800       -1    9.24643   2.19297  -5.95826  L
C-C-0.597300         0     10.48377   2.37897  -5.0532   L
O-O--0.567900        0     11.52034   2.87856  -5.49271  L
C-CT--0.110200       0     9.46992   1.05906  -6.96795  L
C-CT-0.353100        0     8.24281   0.64795  -7.802    L
C-CT--0.412100       0     8.59376  -0.55798  -8.67289  L
C-CT--0.412100       0     7.03084   0.29011  -6.94539  L
H-H-0.271900         0     8.6679    3.39213  -7.65136  L
H-H1-0.092200        0     8.42735   1.89894  -5.30738  L
H-HC-0.045700        0     9.80977   0.18599  -6.41089  L
H-HC-0.045700        0     10.26482   1.36389  -7.64874  L
H-HC--0.036100       0     7.9531    1.45675  -8.45902  L
H-HC-0.100000        0     8.94053  -1.38064  -8.05326  L
H-HC-0.100000        0     9.37603  -0.26927  -9.37599  L
H-HC-0.100000        0     7.72051  -0.86662  -9.24699  L
H-HC-0.100000        0     7.28942  -0.46201  -6.20256  L
H-HC-0.100000        0     6.24705  -0.08301  -7.60093  L
H-HC-0.100000        0     6.65303   1.17981  -6.44416  L
N-N--0.415700        0     10.38575   1.91535  -3.79929  L
C-CT--0.059700       -1    11.53758   1.47602  -2.98874  L
C-C-0.597300         0     11.8847   0.06563  -3.47624  L
O-O--0.567900        0     11.03821  -0.83532  -3.45878  L
C-CT-0.130300        0     11.21227   1.51076  -1.4793   L
C-CT--0.043000       0     10.74717   2.90352  -0.98881  L
C-CT--0.320400       0     12.42087   1.03547  -0.65316  L
C-CT--0.066000       0     11.65122   4.0848   -1.36723  L
H-H-0.271900         0     9.4712    1.56471  -3.53426  L
H-H1-0.086900        0     12.38575   2.13364  -3.18285  L
H-HC-0.018700        0     10.39459   0.81354  -1.28933  L
H-HC-0.023600        0     10.66321   2.88666   0.09718  L
H-HC-0.023600        0     9.7505    3.09566  -1.38516  L
H-HC-0.088200        0     12.64312  -0.00756  -0.87979  L
H-HC-0.088200        0     12.19924   1.11051   0.41154  L
H-HC-0.088200        0     13.29971   1.63976  -0.8809   L
H-HC-0.018600        0     11.29025   4.9869   -0.87463  L
H-HC-0.018600        0     11.62392   4.24652  -2.44446  L
H-HC-0.018600        0     12.67645   3.90186  -1.04708  L
N-N--0.415700        0     13.10577  -0.10749  -3.97105  L
C-CT--0.051800       -1    13.53045  -1.24509  -4.77973  L
C-C-0.597300         0     14.57863  -2.10508  -4.08959  L
O-O--0.567900        0     15.35364  -1.64209  -3.25609  L
C-CT--0.110200       0     14.10042  -0.74582  -6.12989  L
C-CT-0.353100        0     13.14264   0.02051  -7.05743  L
C-CT--0.412100       0     13.93851   0.72906  -8.15441  L
C-CT--0.412100       0     12.16407  -0.92645  -7.74504  L
H-H-0.271900         0     13.71036   0.70786  -3.97203  L
H-H1-0.092200        0     12.66498  -1.87283  -4.98101  L
H-HC-0.045700        0     14.49751  -1.59752  -6.68365  L
H-HC-0.045700        0     14.94155  -0.09428  -5.91812  L
H-HC--0.036100       0     12.59106   0.76562  -6.49209  L
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H-HC-0.100000        0     14.48488   0.00486  -8.75803  L
H-HC-0.100000        0     14.64391   1.42846  -7.70875  L
H-HC-0.100000        0     13.25705   1.28947  -8.7968   L
H-HC-0.100000        0     11.55791  -0.3667   -8.45585  L
H-HC-0.100000        0     11.51461  -1.38041  -7.00136  L
H-HC-0.100000        0     12.70945  -1.69089  -8.2909   L
N-N--0.415700        0     14.65108  -3.35175  -4.52906  L
C-CT--0.025200       -1    15.76273  -4.24056  -4.27356  L
C-C-0.597300         0     15.77268  -5.46723  -5.19453  L
N-N--0.415700        0     16.54237  -6.49116  -4.8142   L
C-CT--0.149000       0     16.76461  -7.71069  -5.58864  L
O-O--0.567900        0     15.10173  -5.49567  -6.23362  L
H-H-0.271900         0     13.9527  -3.65194  -5.20134  L
H-H-0.271900         0     17.01236  -6.40511  -3.91401  L
H-H1-0.069800        0     15.72667  -4.58267  -3.24072  L
H-H1-0.069800        0     16.69828  -3.69966  -4.41932  L
H-H1-0.097600        0     17.39513  -7.48772  -6.45183  L
H-H1-0.097600        0     15.81485  -8.11558  -5.93951  L
H-H1-0.097600        0     17.26748  -8.45552  -4.9686   L
N-N--0.415700        0     13.74322  -4.18485  -8.6084   L
C-CT--0.038900       -1    12.35112  -4.65227  -8.4726   L
C-C-0.597300         0     11.7271  -4.20961  -7.13389  L
O-O--0.567900        0     12.49214  -3.92984  -6.2138   L
C-CT-0.365400        0     12.29326  -6.19077  -8.57798  L
O-OH--0.676100       0     13.06232  -6.8463   -7.58782  L
C-CT--0.243800       0     12.78168  -6.70137  -9.93232  L
H-H-0.271900         0     14.34082  -4.21483  -7.78542  L
H-H-0.271900         0     14.10671  -3.86879  -9.49836  L
H-H1-0.100700        0     11.75591  -4.2254   -9.27931  L
H-H1-0.004300        0     11.26363  -6.51256  -8.4592   L
H-HC-0.064200        0     12.62964  -7.77923  -9.99019  L
H-HC-0.064200        0     13.84272  -6.48786  -10.0639  L
H-HC-0.064200        0     12.21393  -6.22625  -10.73259  L
H-HO-0.410200        0     13.77289  -6.24358  -7.29889  L
N-N--0.254800        0     10.38933  -4.11702  -6.96833  L
C-CT--0.026600       -1    9.77184  -3.63621  -5.72097  L
C-C-0.589600         0     10.16818  -4.49054  -4.51814  L
O-O--0.574800        0     10.01444  -5.71315  -4.52453  L
C-CT--0.007000       0     8.25844  -3.63283  -5.96243  L
C-CT-0.018900        0     8.0778   -4.61444  -7.11561  L
C-CT-0.019200        0     9.35123  -4.43163  -7.93933  L
H-H1-0.064100        0     10.09051  -2.6097   -5.5358   L
H-HC-0.025300        0     7.94131  -2.64175  -6.28043  L
H-HC-0.025300        0     7.69636  -3.93976  -5.07922  L
H-HC-0.021300        0     7.17996  -4.40196  -7.6969   L
H-HC-0.021300        0     8.05073  -5.62753  -6.71571  L
H-H1-0.039100        0     9.56052  -5.34128  -8.49706  L
H-H1-0.039100        0     9.22939  -3.59546  -8.62836  L
N-N--0.415700        0     10.70959  -3.83401  -3.49386  L
C-CT--0.051800       -1    11.16213  -4.47121  -2.26291  L
C-C-0.597300         0     9.99621  -5.08086  -1.4857   L
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 O-O--0.567900        0     8.91517  -4.49347  -1.43618  L
 C-CT--0.110200       0     11.88369  -3.40087  -1.42125  L
 C-CT-0.353100        0     12.8315  -3.98118  -0.35705  L
 C-CT--0.412100       0     14.15379  -4.41226  -0.99194  L
 C-CT--0.412100       0     13.13067  -2.91645   0.69275  L
 H-H-0.271900         0     10.79439  -2.82665  -3.56401  L
 H-H1-0.092200        0     11.86517  -5.26     -2.52719  L
 H-HC-0.045700        0     11.12707  -2.78185  -0.93656  L
 H-HC-0.045700        0     12.46541  -2.74882  -2.07401  L
 H-HC--0.036100       0     12.36969  -4.83369   0.13938  L
 H-HC-0.100000        0     14.61783  -3.56135  -1.48888  L
 H-HC-0.100000        0     13.98137  -5.21048  -1.7123   L
 H-HC-0.100000        0     14.84412  -4.7734   -0.23328  L
 H-HC-0.100000        0     13.56762  -2.03693   0.2221   L
 H-HC-0.100000        0     13.82563  -3.30538   1.43534  L
 H-HC-0.100000        0     12.20125  -2.64272   1.19028  L
 N-N--0.415700        0     10.22797  -6.2442   -0.87866  L
 C-CT--0.024900      -1     9.25453  -6.94159  -0.04411  L
 C-C-0.597300         0     9.92472  -7.93176   0.91746  L
 O-O--0.567900        0     11.13683  -7.90533   1.14812  L
 C-CT-0.211700        0     8.21603  -7.59601  -0.97492  L
 O-OH--0.654600       0     7.12479  -8.13125  -0.24824  L
 H-H-0.271900         0     11.13094  -6.69045  -1.00441  L
 H-H1-0.084300        0     8.73548  -6.20026   0.5653   L
 H-H1-0.035200        0     8.69665  -8.39196  -1.54579  L
 H-H1-0.035200        0     7.83395  -6.85043  -1.67276  L
 H-HO-0.427500        0     6.34127  -7.53591  -0.31406  L
 N-N--0.347900        0     9.10802  -8.79097   1.52205  L
 C-CT--0.240000      -1     9.44429  -9.83682   2.48301  L
 C-C-0.734100         0     10.37231  -10.90915   1.89907  L
 O-O--0.589400        0     11.33567  -11.29224   2.55633  L
 C-CT--0.009400       0     8.12803  -10.40112   3.07735  L
 C-CT-0.018700        0     7.19201  -9.32364   3.70115  L    H-HC
1455  0.        0.
 C-CT--0.047900       0     5.82541  -9.16709   2.99714  H
 C-CT--0.014300       0     5.04951  -7.90705   3.40236  H
 N-N3--0.385400       0     3.70874  -7.80978   2.78459  H
 H-H-0.274700         0     8.14417  -8.72027   1.21316  L
 H-H1-0.142600        0     10.0085  -9.37853   3.29766  L
 H-HC-0.036200        0     8.39192  -11.11654   3.85804  L
 H-HC-0.036200        0     7.58804  -10.95337   2.30711  L
 H-HC-0.010300        0     7.69645  -8.35634   3.7102   L
 H-HC-0.010300        0     7.00411  -9.58847   4.74278  L
 H-HC-0.062100        0     5.22536  -10.05765   3.21456  H
 H-HC-0.062100        0     5.98872  -9.14596   1.91608  H
 H-HP-0.113500        0     5.59963  -7.00977   3.11302  H
 H-HP-0.113500        0     4.90564  -7.85222   4.48492  H
 H-H-0.340000         0     3.7758   -8.03407   1.78703  H
 H-H-0.340000         0     2.57514  -6.40469   2.78967  H
 H-H-0.340000         0     3.12341  -8.57514   3.14578  H
 N-N--0.347900        0     10.1477  -11.27435   0.62999  L
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C-CT--0.263700       -1    11.07642  -11.85844  -0.36728  L
C-C-0.734100         0     12.56923  -11.58715  -0.12879  L
O-O--0.589400        0     13.39081  -12.45318  -0.40313  L
C-CT--0.000700       0     10.60504  -11.33022  -1.73433  L
C-CT-0.039000        0     11.54594  -11.57308  -2.92457  L
C-CT-0.048600        0     10.8854   -10.98562  -4.17654  L
N-N2--0.529500       0     11.84695  -10.76424  -5.27303  L
C-CA-0.807600        0     11.76973  -9.80916   -6.18528  L
N-N2--0.862700       0     10.79107  -8.95707   -6.23119  L
N-N2--0.862700       0     12.70413  -9.6649    -7.07723  L
H-H-0.274700         0     9.23905   -10.98127   0.27884  L
H-H1-0.156000        0     10.97038  -12.94441  -0.35752  L
H-HC-0.032700        0     10.45688  -10.25148  -1.6471   L
H-HC-0.032700        0     9.63542   -11.77956  -1.958    L
H-HC-0.028500        0     11.72468  -12.6407   -3.05886  L
H-HC-0.028500        0     12.49331  -11.06105  -2.7504   L
H-H1-0.068700        0     10.44416  -10.03184  -3.89425  L
H-H1-0.068700        0     10.08263  -11.64749  -4.50837  L
H-H-0.345600         0     12.63821  -11.38175  -5.318    L
H-H-0.447800         0     10.59549  -8.40528   -7.05856  L
H-H-0.447800         0     10.07052  -8.96001   -5.51073  L
H-H-0.447800         0     12.70821  -8.78034   -7.57466  L
H-H-0.447800         0     13.47489  -10.29974  -7.14472  L
N-N--0.415700        0     12.92547  -10.37885   0.30231  L
C-CT--0.058100       -1    14.29958  -9.87611    0.38527  L
C-C-0.597300         0     14.91789  -9.88754    1.79169  L
N-N--0.415700        0     14.2043   -10.39953   2.80254  L
C-CT--0.149000       0     14.66769  -10.53147   4.18151  L
O-O--0.567900        0     16.0494   -9.42161    1.94581  L
C-CT--0.007400       0     14.26376  -8.44216   -0.17731  L
C-CC-0.186800        0     13.72004  -8.27138   -1.57889  L
N-NB--0.543200       0     12.37443  -8.10038   -1.90662  L
C-CW--0.220700       0     14.46754  -8.09576   -2.70575  L
C-CR-0.163500        0     12.33769  -7.83576   -3.22036  L
N-NA--0.279500       0     13.58163  -7.81857   -3.72842  L
H-H-0.271900         0     12.1795   -9.71369    0.4544   L
H-H-0.271900         0     13.28196  -10.76107   2.57787  L
H-H1-0.136000        0     14.95188  -10.47903  -0.24879  L
H-HC-0.036700        0     15.26032  -8.00823   -0.14683  L
H-HC-0.036700        0     13.62877  -7.85437    0.47723  L
H-H4-0.186200        0     15.54842  -8.11095   -2.74795  L
H-H-0.333900         0     13.80923  -7.57222   -4.68339  L
H-H5-0.143500        0     11.43489  -7.63059   -3.78119  L
H-H1-0.097600        0     15.38773  -9.7464     4.41731  L
H-H1-0.097600        0     15.1511   -11.50154   4.3114   L
H-H1-0.097600        0     13.81821  -10.46363   4.86266  L
N-N--0.415700        0     14.58948  -6.8755     5.3961   L
C-CT--0.038900       -1    13.91006  -5.68584    4.85059  L
C-C-0.597300         0     12.7368   -5.16898    5.69575  L
O-O--0.567900        0     12.18682  -4.10064    5.41146  L
C-CT-0.365400        0     13.40269  -5.95373    3.42558  L
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O-OH--0.676100       0     12.70766  -7.18332   3.38526  L
C-CT--0.243800       0     14.58065  -6.02071   2.46135  L
H-H-0.271900         0     14.3705   -7.75852   4.94567  L
H-H-0.271900         0     15.38547  -6.78742   6.01492  L
H-H1-0.100700        0     14.62544  -4.86532   4.80425  L
H-H1-0.004300        0     12.7406   -5.14691   3.10855  L
H-HC-0.064200        0     14.19869  -6.05451   1.44889  L
H-HC-0.064200        0     15.18638  -6.9059    2.6559   L
H-HC-0.064200        0     15.19977  -5.12938   2.56274  L
H-HO-0.410200        0     12.29801  -7.29591   2.5107   L
N-N--0.415700        0     12.36486  -5.89337   6.75364  L
C-CT--0.024900       -1    11.46181  -5.42186   7.80902  L
C-C-0.597300         0     11.99257  -4.15707   8.47995  L
O-O--0.567900        0     13.19452  -4.05251   8.7122   L
C-CT-0.211700        0     11.28236  -6.51533   8.86444  L
O-OH--0.654600       0     12.54383  -6.96521   9.32223  L
H-H-0.271900         0     12.87976  -6.74151   6.94022  L
H-H1-0.084300        0     10.49616  -5.21285   7.3614   L
H-H1-0.035200        0     10.74316  -7.35554   8.42478  L
H-H1-0.035200        0     10.70197  -6.12552   9.70238  L
H-HO-0.427500        0     13.074    -6.19378   9.57236  L
N-N--0.415700        0     11.09731  -3.23344   8.83559  L
C-CT--0.087500       -1    11.43898  -2.01007   9.59004  L
C-C-0.597300         0     12.13684  -2.32447   10.92207  L
N-N--0.415700        0     11.64063  -3.3293    11.66245  L
O-O--0.567900        0     13.08784  -1.63729   11.28465  L
C-CT-0.298500        0     10.18943  -1.15455   9.85001  L
C-CT--0.319200       0     10.47277   0.11684   10.66362  L
C-CT--0.319200       0     9.57659   -0.69969   8.52745  L
H-H-0.271900         0     10.12569  -3.4303    8.6234   L
H-H-0.096900         0     10.84927  -3.84086   11.30333  L
H-H1-0.096900        0     12.1446   -1.42393   9.001    L
H-HC--0.029700       0     9.44964   -1.75141   10.38573  L
H-HC-0.079100        0     9.5694     0.71965   10.75069  L
H-HC-0.079100        0     11.25624   0.70271   10.18141  L
H-HC-0.079100        0     10.8009   -0.14545   11.66997  L
H-HC-0.079100        0     9.29748   -1.55523   7.91542  L
H-HC-0.079100        0     10.28162  -0.07493   7.97977  L
H-HC-0.079100        0     8.6844    -0.13053   8.75965  L
N-N--0.415700        0     14.07483   7.09525   5.64534  L
C-CT--0.051800       -1    13.45915   6.44274   4.48192  L
C-C-0.597300         0     12.90781   7.42619   3.4308   L
O-O--0.567900        0     12.65278   7.01612   2.30472  L
C-CT--0.110200       0     12.34397   5.48384   4.94587  L
C-CT-0.353100        0     12.76637   4.37372   5.92794  L
C-CT--0.412100       0     11.54593   3.52698   6.28978  L
C-CT--0.412100       0     13.83798   3.45842   5.33368  L
H-H-0.271900         0     13.57456   7.11113   6.52615  L
H-H-0.271900         0     15.07296   7.27104   5.64424  L
H-H1-0.092200        0     14.22281   5.85425   3.97194  L
H-HC-0.045700        0     11.92793   5.00565   4.05898  L
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H-HC-0.045700        0     11.54932   6.0713    5.40712  L
H-HC--0.036100       0     13.15266   4.82309   6.84277  L
H-HC-0.100000        0     11.83087   2.75597   7.00587  L
H-HC-0.100000        0     11.1391   3.05641   5.39571  L
H-HC-0.100000        0     10.77914   4.15553   6.74239  L
H-HC-0.100000        0     14.02388   2.62216   6.00872  L
H-HC-0.100000        0     14.77128   4.00582   5.21073  L
H-HC-0.100000        0     13.51176   3.07609   4.36682  L
N-N--0.415700        0     12.73889   8.70716   3.77341  L
C-CT-0.033700        0     12.38176   9.77159   2.82775  L
C-C-0.597300         0     13.53358   10.09962   1.8509   L
N-N--0.415700        0     14.74747   10.31758   2.37715  L
C-CT--0.149000       -1    15.9687   10.59313   1.61887  L
O-O--0.567900        0     13.32684   10.14914   0.6395   L
C-CT--0.182500       0     11.94034   11.00567   3.6254   L
H-H-0.271900         0     12.91968   8.9586    4.73145  L
H-H-0.271900         0     14.8086   10.30637   3.38228  L
H-H1-0.082300        0     11.53474   9.43689   2.22463  L
H-HC-0.060300        0     12.7541   11.3708   4.25318  L
H-HC-0.060300        0     11.0832   10.75614   4.25265  L
H-HC-0.060300        0     11.64441   11.79741   2.93465  L
H-H1-0.097600        0     15.72581   10.97403   0.62417  L
H-H1-0.097600        0     16.55823   9.68101   1.5229   L
H-H1-0.097600        0     16.5652   11.34674   2.13694  L
N-N--0.415700        0     14.85524   7.14374   0.54359  L
C-CT--0.051800       -1    15.12581   7.83816  -0.71158  L
C-C-0.597300         0     13.85502   8.0163   -1.55807  L
O-O--0.567900        0     12.81689   7.41499  -1.28224  L
C-CT--0.110200       0     16.19315   7.04026  -1.49572  L
C-CT-0.353100        0     17.59254   6.99173  -0.85482  L
C-CT--0.412100       0     18.45707   5.96936  -1.59122  L
C-CT--0.412100       0     18.2982   8.34692  -0.92702  L
H-H-0.271900         0     13.88651   7.13329   0.86404  L
H-H-0.271900         0     15.48363   6.41795   0.85363  L
H-H1-0.092200        0     15.50348   8.83529  -0.49227  L
H-HC-0.045700        0     16.30029   7.46235  -2.49521  L
H-HC-0.045700        0     15.82972   6.01769  -1.61268  L
H-HC--0.036100       0     17.51003   6.68528   0.18816  L
H-HC-0.100000        0     19.44459   5.91899  -1.13174  L
H-HC-0.100000        0     18.56805   6.24968  -2.63915  L
H-HC-0.100000        0     18.00013   4.98057  -1.53538  L
H-HC-0.100000        0     18.41016   8.65944  -1.96591  L
H-HC-0.100000        0     19.28895   8.26705  -0.47788  L
H-HC-0.100000        0     17.73634   9.10228  -0.38385  L
N-N--0.415700        0     13.95873   8.80783  -2.62641  L
C-CT--0.025200       -1    12.9495   8.95097  -3.67885  L
C-C-0.597300         0     12.93218   10.36595  -4.26531  L
N-N--0.415700        0     12.67037   10.48745  -5.57136  L
C-CT--0.149000       0     12.61463   11.76581  -6.2797   L
O-O--0.567900        0     13.14099   11.33232  -3.53325  L
H-H-0.271900         0     14.81158   9.33639  -2.73315  L
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H-H-0.271900          0     12.52202   9.64631  -6.10698  L
H-H1-0.069800         0     11.95802   8.74385  -3.28045  L
H-H1-0.069800         0     13.15703   8.23526  -4.47356  L
H-H1-0.097600         0     11.84138   12.40095  -5.84229  L
H-H1-0.097600         0     12.39073   11.6061  -7.33592  L
H-H1-0.097600         0     13.57426   12.28044  -6.1939   L
N-N--0.415700         0     12.21029   5.48818  -9.5554   L
C-CT--0.025200       -1     12.32964   4.64798  -8.36704  L
C-C-0.597300          0     13.75728   4.6161   -7.81372  L
O-O--0.567900         0     14.67002   5.18451  -8.41099  L
H-H-0.271900          0     11.40645   5.36698  -10.17128  L
H-H-0.271900          0     13.06577   5.88722  -9.92318  L
H-H1-0.069800         0     12.03823   3.62789  -8.61555  L
H-H1-0.069800         0     11.66671   5.01241  -7.58582  L
N-N--0.415700         0     13.9548   3.9934   -6.64821  L
C-CT--0.087500       -1     15.21716   4.04691  -5.8844   L
C-C-0.597300          0     15.50303   2.75554  -5.12117  L
O-O--0.567900         0     14.61629   2.17273  -4.50471  L
C-CT-0.298500         0     15.21461   5.21808  -4.87709  L
C-CT--0.319200        0     15.34713   6.57824  -5.57156  L
C-CT--0.319200        0     13.96283   5.24887  -3.98892  L
H-H-0.271900          0     13.15606   3.53353  -6.2149   L
H-H1-0.096900         0     16.04204   4.20334  -6.58033  L
H-HC--0.029700        0     16.08515   5.10764  -4.22892  L
H-HC-0.079100         0     16.21152   6.56812  -6.23674  L
H-HC-0.079100         0     15.48882   7.3625   -4.8302   L
H-HC-0.079100         0     14.45593   6.79496  -6.15951  L
H-HC-0.079100         0     14.03588   6.067    -3.28543  L
H-HC-0.079100         0     13.88196   4.32498  -3.41992  L
H-HC-0.079100         0     13.06108   5.37902  -4.58709  L
N-N--0.415700         0     16.75649   2.30405  -5.13775  L
C-CT--0.059700       -1     17.19757   1.08798  -4.4394   L
C-C-0.597300          0     17.4029   1.34781  -2.94886  L
O-O--0.567900         0     17.98137   2.35567  -2.54101  L
C-CT-0.130300         0     18.46572   0.50827  -5.11683  L
C-CT--0.043000        0     18.14098   0.10068  -6.57728  L
C-CT--0.320400        0     19.00797  -0.7113   -4.34373  L
C-CT--0.066000        0     19.36603  -0.28358  -7.41748  L
H-H-0.271900          0     17.45116   2.84903  -5.62466  L
H-H1-0.086900         0     16.41846   0.33552  -4.51883  L
H-HC-0.018700         0     19.23774   1.28021  -5.12805  L
H-HC-0.023600         0     17.66256   0.93334  -7.09247  L
H-HC-0.023600         0     17.43849  -0.73415  -6.57427  L
H-HC-0.088200         0     19.88433  -1.12352  -4.84168  L
H-HC-0.088200         0     18.2428  -1.48473  -4.26595  L
H-HC-0.088200         0     19.33008  -0.42094  -3.34366  L
H-HC-0.018600         0     20.11445   0.50814  -7.36901  L
H-HC-0.018600         0     19.06084  -0.41743  -8.45571  L
H-HC-0.018600         0     19.79851  -1.21922  -7.06499  L
N-N--0.415700         0     16.94039   0.40623  -2.13093  L
C-CT--0.002400       -1     17.22731   0.35757  -0.71038  L
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C-C-0.597300          0     18.68915  -0.06449  -0.4359   L
N-N--0.415700         0     19.59972   0.91961  -0.38178  L
C-CT--0.149000        -1    21.02573   0.75326  -0.0769   L
O-O--0.567900         0     18.98712  -1.24791  -0.28571  L
C-CT--0.034300        0     16.19693  -0.53804  -0.00743  L
C-CA-0.011800         0     16.30435  -0.49975   1.50555  L
C-CA--0.125600        0     15.95138   0.66985   2.20743  L
C-CA--0.125600        0     16.79365  -1.61488   2.21115  L
C-CA--0.170400        0     16.09314   0.72497   3.60627  L
C-CA--0.170400        0     16.92466  -1.56351   3.61047  L
C-CA--0.107200        0     16.57665  -0.39358   4.30792  L
H-H-0.271900          0     16.46197  -0.39012  -2.53945  L
H-H-0.271900          0     19.26624   1.83656  -0.64722  L
H-H1-0.097800         0     17.10504   1.36349  -0.30875  L
H-HC-0.029500         0     16.30802  -1.56482  -0.36056  L
H-HC-0.029500         0     15.19688  -0.20339  -0.28414  L
H-HA-0.133000         0     15.58037   1.53042   1.67075  L
H-HA-0.133000         0     17.09476  -2.5041    1.67445  L
H-HA-0.143000         0     15.83569   1.62464   4.14514  L
H-HA-0.143000         0     17.31545  -2.41647   4.14764  L
H-HA-0.129700         0     16.69271  -0.35367   5.38255  L
H-H1-0.097600         0     21.473    0.05008  -0.7824   L
H-H1-0.097600         0     21.14314   0.35429   0.93249  L
H-H1-0.097600         0     21.54274   1.7111   -0.14947  L
C-CT-0.055800         0    -6.82286  -9.78275  -6.52964  L
C-CT-0.106500         0    -6.20139  -10.8811  -5.66645  L
O-OS--0.354800        0    -4.97976  -11.30543  -6.25274  L
C-CT-0.202200         0    -5.83728  -10.49177  -4.22673  L
O-OS--0.495400        0    -6.90102  -10.47873  -3.2888   L
C-CT-0.067000         0    -4.88684  -11.6512  -3.91056  L
O-OH--0.613900        0    -5.58608  -12.87723  -3.69428  L
C-CT-0.006600         0    -4.11041  -11.78117  -5.22501  L
N-N*--0.048400        0    -2.82561  -11.01491  -5.21456  L
C-C-0.753800          0    -1.66805  -11.66065  -4.77115  L
O-O--0.625800         0    -1.68563  -12.80384  -4.31395  L
N-NC--0.758400        0    -0.46409  -10.99057  -4.85739  L
C-CA--0.521500        0    -0.38272  -9.78106  -5.35393  L
N-N2--0.953800        0     0.80301  -9.31279  -5.62069  L
C-CM--0.521500        0    -1.52743  -9.09702  -5.80599  L
C-CM-0.005300         0    -2.72652  -9.73589  -5.71873  L
H-HC-0.067900         0    -7.8114   -9.5291   -6.15951  L
H-HC-0.067900         0    -6.19004  -8.89938  -6.52236  L
H-H1-0.117400         0    -6.87958  -11.73429  -5.63157  L
H-H1-0.061500         0    -5.2698   -9.56132  -4.21018  L
H-H1-0.097200         0    -4.22915  -11.42011  -3.07239  L
H-HO-0.418600         0    -5.76947  -12.99646  -2.73303  L
H-H2-0.202900         0    -3.8819   -12.84052  -5.38096  L
H-H-0.423900          0     1.65396  -9.83423  -5.41093  L
H-H-0.423900          0     0.93149  -8.48469  -6.20042  L
H-HA-0.192800         0    -1.49302  -8.1082   -6.24396  L
H-H4-0.195800         0    -3.61353  -9.2487   -6.09548  L
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 P-P-1.166200          0    -7.62018  -9.14156  -2.82116  L
 O-O2--0.776000        0    -8.38606  -9.51838  -1.61666  L
 O-O2--0.776000        0    -8.37195  -8.60458  -3.96808  L
 O-OS--0.498900        0    -6.45488  -8.10446  -2.44143  L
 C-CT-0.055800         0    -5.62333  -8.22846  -1.2881   L    H-H1
1732  0.        0.
 C-CT-0.106500         0    -4.44606  -7.22281  -1.31097  H
 O-OS--0.354800        0    -3.65563  -7.54738  -2.45235  H
 C-CT-0.202200         0    -4.82723  -5.75952  -1.54     H
 O-OH--0.654100        0    -5.24721  -5.02542  -0.43261  H
 C-CT-0.067000         0    -3.63044  -5.15202  -2.28364  H
 O-OH--0.613900        0    -2.5266   -4.65271  -1.536    H
 C-CT-0.039400         0    -3.10853  -6.39423  -3.04013  H
 N-N*--0.025100        0    -3.48866  -6.38034  -4.43601  H
 C-CK-0.200600         0    -4.6321   -6.89112  -5.01032  H
 N-NB--0.607300        0    -4.67563  -6.75228  -6.30825  H
 C-CB-0.051500         0    -3.49895  -6.09563  -6.60937  H
 C-CA-0.700900         0    -2.88677  -5.71585  -7.81944  H
 N-N2--0.901900        0    -3.43971  -5.99359  -9.02837  H
 N-NC--0.761500        0    -1.74548  -5.01004  -7.77467  H
 C-CQ-0.587500         0    -1.17342  -4.80138  -6.58347  H
 N-NC--0.699700        0    -1.5739   -5.21559  -5.38059  H
 C-CB-0.305300         0    -2.75402  -5.84157  -5.46006  H
 H-H1-0.067900         0    -5.2191   -9.24035  -1.23064  L
 H-H1-0.067900         0    -6.22462  -8.04022  -0.40155  L
 H-H1-0.117400         0    -3.86314  -7.31749  -0.38453  H
 H-H1-0.061500         0    -5.56863  -5.76434  -2.33389  H
 H-HO-0.437600         0    -6.17544  -5.25489  -0.21897  H
 H-H1-0.097200         0    -3.96576  -4.3797   -2.98167  H
 H-HO-0.418600         0    -0.80323  -5.64541  -0.24188  H
 H-H2-0.200700         0    -2.01858  -6.40349  -2.97545  H
 H-H5-0.155300         0    -5.38564  -7.36339  -4.39931  H
 H-H-0.411500          0    -2.78037  -5.99118  -9.79406  H
 H-H-0.411500          0    -4.057    -6.79559  -9.03097  H
 H-H5-0.047300         0    -0.26545  -4.20908  -6.58948  H
 C-CQ-0.587500         0     6.61419   1.83558  -3.07889  L
 P-P-1.166200          0     0.94059  -3.01352   1.27883  H
 N-N3-0.001700         0    -3.80405  -2.97466   0.62643  H
 C-CT-0.058800         0    -3.51631  -2.53209  -0.74869  H
 C-CT-0.090900         0    -3.28322  -1.01865  -0.73946  H
 C-CT--0.023600        0    -2.81689  -0.35001  -2.04566  H
 C-C-0.808700          0    -3.24021   1.11712  -2.0091   H
 O-O2--0.818900        0    -2.50411   1.93329  -1.41904  H
 O-O2--0.818900        0    -4.3795    1.39134  -2.54151  H
 C-C-0.562100          0    -2.3406   -3.313    -1.30706  H
 O-O--0.588900         0    -1.23487  -2.86117  -1.46981  H
 O-OS--0.421000        0    -0.56148  -3.08109   1.31282  H
 O-O2--0.776000        0     1.65233  -3.97736   0.27917  H
 O-O2--0.776000        0     1.59442  -3.28301   2.6987   H
 O-OS--0.498900        0     1.49373  -1.59448   0.85011  H
 C-CT-0.055800         0     1.19782  -0.48162   1.6987   H
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 C-CT-0.106500        0     1.36231   0.81895   0.89719  L    H-H1
1776  0.        0.
 O-OS--0.354800       0     2.72654   1.09923   0.59747  L
 C-CT-0.039400        0     2.93763   1.07352  -0.81474  L
 N-N*--0.025100       0     4.12126   0.22557  -1.10803  L
 C-CB-0.305300        0     5.22631   0.5997   -1.84233  L
 N-NC--0.699700       0     5.41138   1.76337  -2.52133  L
 N-NC--0.761500       0     7.59495   0.93797  -3.04867  L
 C-CA-0.700900        0     7.35323  -0.20739  -2.40944  L
 N-N2--0.901900       0     8.34277  -1.08249  -2.46004  L
 C-CB-0.051500        0     6.1297   -0.42351  -1.72927  L
 N-NB--0.607300       0     5.60969  -1.46766  -0.95491  L
 C-CK-0.200600        0     4.41919  -1.02818  -0.62663  L
 C-CT-0.067000        0     1.64356   0.60587  -1.48596  L
 O-OH--0.613900       0     1.42425   1.31432  -2.70443  L
 C-CT-0.202200        0     0.56715   0.86537  -0.41239  L
 O-OH--0.654100       0    -0.04897   2.14885  -0.47427  L
 H-H5-0.047300        0     6.82154   2.74628  -3.62365  L
 H-H-0.239100         0    -3.09943  -2.59254   1.26469  H
 H-H-0.239100         0    -3.7904   -3.98914   0.71295  H
 H-H-0.239100         0    -5.41768  -2.42812   0.77498  H
 H-HP-0.120200        0    -4.40444  -2.77591  -1.3458   H
 H-HC--0.023200       0    -2.5256   -0.78634   0.01258  H
 H-HC--0.023200       0    -4.23917  -0.59181  -0.42109  H
 H-HC--0.031500       0    -3.24338  -0.83598  -2.9238   H
 H-HC--0.031500       0    -1.73126  -0.40904  -2.11854  H
 H-H1-0.067900        0     1.87325  -0.48712   2.55975  H
 H-H1-0.067900        0     0.15792  -0.54189   2.04367  H
 H-H1-0.117400        0     0.98945   1.61946   1.53314  L
 H-H2-0.200700        0     3.13827   2.08401  -1.18108  L
 H-H-0.411500         0     8.16865  -2.02574  -2.14291  L
 H-H-0.411500         0     9.17768  -0.84076  -2.97797  L
 H-H5-0.155300        0     3.72791  -1.59626  -0.01822  L
 H-H1-0.097200        0     1.69018  -0.46954  -1.66739  L
 H-HO-0.418600        0     1.94846   0.89638  -3.4358   L
 H-H1-0.061500        0    -0.19337   0.08361  -0.43672  L
 H-HO-0.437600        0    -0.90417   2.04589  -0.95499  L
 O-OW--0.834000       0     6.22415   3.76334  -0.38608  L
 H-HW-0.417000        0     5.27184   3.85405  -0.20745  L
 H-HW-0.417000        0     6.47312   3.07717   0.25825  L
 O-OW--0.834000       0     11.62401   11.09635  -1.24665  L
 H-HW-0.417000        0     12.30922   10.93819  -0.57445  L
 H-HW-0.417000        0     12.12897   11.46168  -1.99297  L
 O-OW--0.834000       0     10.47662   8.68311  -1.13723  L
 H-HW-0.417000        0     10.70994   9.63665  -1.14536  L
 H-HW-0.417000        0     11.35171   8.25879  -1.0387   L
 O-OW--0.834000       0     8.21157   7.27759  -11.85276  L
 H-HW-0.417000        0     7.5285    7.5923   -12.44409  L
 H-HW-0.417000        0     7.81518   6.44956  -11.48494  L
 O-OW--0.834000       0     17.8153  -8.26267   0.14637  L
 H-HW-0.417000        0     18.64899  -8.68421   0.3715   L
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H-HW-0.417000        0     17.20745  -8.61531   0.82249  L
O-OW--0.834000       0     17.4611   -6.49026  -1.95078  L
H-HW-0.417000        0     17.53254  -7.18149  -1.26208  L
H-HW-0.417000        0     17.99525  -5.78073  -1.58541  L
O-OW--0.834000       0     10.2765    2.53797  -10.16003  L
H-HW-0.417000        0     9.40079    2.84519  -9.83707  L
H-HW-0.417000        0     10.48172    3.21468  -10.81753  L
O-OW--0.834000       0     6.37821   -7.81514  -3.61274  L
H-HW-0.417000        0     5.55179   -8.3193   -3.50853  L
H-HW-0.417000        0     6.08279   -6.88997  -3.51372  L
O-OW--0.834000       0     2.37969   -4.37973  -5.43456  L
H-HW-0.417000        0     2.13976   -4.19429  -6.36848  L
H-HW-0.417000        0     2.59879   -3.47964  -5.09923  L
O-OW--0.834000       0     9.95741    5.12661  -11.35039  L
H-HW-0.417000        0     9.06271    4.84437  -11.06499  L
H-HW-0.417000        0     9.75135    5.97168  -11.77686  L
O-OW--0.834000       0    -1.80202   -8.94281  -8.67077  L
H-HW-0.417000        0    -1.15154   -9.57851  -8.99016  L
H-HW-0.417000        0    -1.73945   -9.07996  -7.71082  L
O-OW--0.834000       0    -0.04476   -7.26262  -4.10654  L
H-HW-0.417000        0    -0.62823   -6.74437  -4.67756  L
H-HW-0.417000        0    -0.01186   -8.14304  -4.5917   L
O-OW--0.834000       0     3.90178   -8.98554  -3.48419  L
H-HW-0.417000        0     3.13323   -9.58403  -3.33993  L
H-HW-0.417000        0     3.45758   -8.12011  -3.60902  L
O-OW--0.834000       0     0.38342   -4.32217  -3.48028  L
H-HW-0.417000        0     1.11417   -4.34718  -4.11991  L
H-HW-0.417000        0    -0.35252   -4.70414  -3.98132  L
O-OW--0.834000       0     0.01034   -5.66637  -0.80078  H
H-HW-0.417000        0    -0.24833   -5.09877  -1.55397  H
H-HW-0.417000        0     1.02198   -4.68368  -0.07764  H
O-OW--0.834000       0     5.49251   -5.2365   -3.68337  L
H-HW-0.417000        0     5.27585   -5.49982  -4.5985   L
H-HW-0.417000        0     5.53269   -4.25892  -3.75381  L
O-OW--0.834000       0    -6.51211   -8.75631   2.01841  L
H-HW-0.417000        0    -6.37526   -7.93482   2.53229  L
H-HW-0.417000        0    -7.1567    -8.4813    1.35072  L
O-OW--0.834000       0     4.75372  -10.44515  -1.08701  L
H-HW-0.417000        0     4.04338  -10.10355  -0.51739  L
H-HW-0.417000        0     4.57467  -10.01699  -1.9359   L
O-OW--0.834000       0     2.54612   -6.69428  -3.86985  L
H-HW-0.417000        0     1.5915    -6.91359  -3.96131  L
H-HW-0.417000        0     2.6178    -5.85657  -4.36185  L
O-OW--0.834000       0     4.83585   -6.78677  -0.04031  L
H-HW-0.417000        0     3.97012   -7.03591  -0.41045  L
H-HW-0.417000        0     4.8757    -5.8433   -0.28996  L
O-OW--0.834000       0     4.73579   -6.05064  -6.18451  L
H-HW-0.417000        0     4.43647   -6.97992  -6.23855  L
H-HW-0.417000        0     3.90907   -5.54896  -6.21713  L
O-OW--0.834000       0     3.41816   -5.61294   5.40307  L
H-HW-0.417000        0     2.57392   -5.13265   5.48649  L
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H-HW-0.417000        0     3.31114  -6.37325   5.99517  L
O-OW--0.834000       0     5.23143  -2.59016  -3.66135  L
H-HW-0.417000        0     4.35059  -2.29314  -3.96456  L
H-HW-0.417000        0     5.25404  -2.28739  -2.73935  L
O-OW--0.834000       0     0.68308  -13.87194  -3.51895  L
H-HW-0.417000        0    -0.20608  -13.6292  -3.84406  L
H-HW-0.417000        0     1.25106  -13.57289  -4.25081  L
O-OW--0.834000       0     4.54057  -4.3697   -1.14232  L
H-HW-0.417000        0     4.87445  -4.66567  -2.00799  L
H-HW-0.417000        0     3.74177  -3.85289  -1.39018  L
O-OW--0.834000       0     2.71076  -9.19481   0.35105  L
H-HW-0.417000        0     1.82948  -9.57386   0.44557  L
H-HW-0.417000        0     2.54853  -8.44612  -0.25991  L
O-OW--0.834000       0     0.03425  -10.93188  -7.76644  L
H-HW-0.417000        0    -0.05768  -10.43456  -6.89404  L
H-HW-0.417000        0    -0.47135  -11.72499  -7.57633  L
O-OW--0.834000       0     7.41568  -10.81342  -0.39116  L
H-HW-0.417000        0     7.286    -9.85181  -0.46097  L
H-HW-0.417000        0     6.53544  -11.13429  -0.65066  L
O-OW--0.834000       0     4.21989  -3.90083   1.54563  L
H-HW-0.417000        0     3.2525   -3.893     1.47429  L
H-HW-0.417000        0     4.47292  -4.03238   0.61429  L
O-OW--0.834000       0     2.44438  -2.90081  -2.13317  H
H-HW-0.417000        0     1.54658  -3.27956  -2.20662  H
H-HW-0.417000        0     2.50722  -2.45925  -3.02188  H
O-OW--0.834000       0     8.92402  -8.16269  -4.30985  L
H-HW-0.417000        0     7.97175  -8.1159   -4.06966  L
H-HW-0.417000        0     9.17672  -7.22156  -4.35189  L
O-OW--0.834000       0     4.25517  -8.77383  -6.31873  L
H-HW-0.417000        0     3.72742  -9.45504  -6.78289  L
H-HW-0.417000        0     4.24326  -9.07754  -5.39601  L
O-OW--0.834000       0     1.64899  -3.81765  -7.98964  L
H-HW-0.417000        0     1.37192  -2.88412  -8.09341  L
H-HW-0.417000        0     1.2249   -4.25215  -8.73333  L
O-OW--0.834000       0     2.85253  -1.50441   4.63944  H
H-HW-0.417000        0     2.15084  -2.10562   4.3529   H
H-HW-0.417000        0     3.61932  -2.10926   4.57377  H
O-OW--0.834000       0     1.81014  -12.30182  -5.46981  L
H-HW-0.417000        0     2.21279  -11.90527  -6.25501  L
H-HW-0.417000        0     0.96461  -11.79229  -5.37866  L
O-OW--0.834000       0     6.68571  -7.77561  -7.39585  L
H-HW-0.417000        0     6.31254  -6.94951  -7.05323  L
H-HW-0.417000        0     6.016    -8.41884  -7.11406  L
O-OW--0.834000       0     2.36766  -7.03111  -1.19331  L
H-HW-0.417000        0     1.62628  -6.42112  -1.02558  L
H-HW-0.417000        0     2.53143  -6.88994  -2.1473   L
O-OW--0.834000       0     1.76698  -10.5344  -3.28531  L
H-HW-0.417000        0     1.97882  -11.4221  -3.60941  L
H-HW-0.417000        0     0.99844  -10.299   -3.86797  L
O-OW--0.834000       0    -7.92354  -5.52741   0.09092  L
H-HW-0.417000        0    -8.45313  -4.91105   0.62831  L
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H-HW-0.417000        0    -8.3291   -6.3873    0.28843  L
O-OW--0.834000       0     2.71733  -10.66704  -7.60709  L
H-HW-0.417000        0     2.97085  -11.06435  -8.44519  L
H-HW-0.417000        0     1.73751  -10.61866  -7.68201  L
O-OW--0.834000       0    -3.51527  -2.96722  -13.2585  L
H-HW-0.417000        0    -3.20476  -3.87771  -13.24056  L
H-HW-0.417000        0    -3.60266  -2.76898  -12.30186  L
O-OW--0.834000       0     9.19854  -8.01041  -8.39821  L
H-HW-0.417000        0     8.92639  -8.35756  -9.25063  L
H-HW-0.417000        0     8.33807  -7.89978  -7.93712  L
O-OW--0.834000       0     1.7731   -5.79806   2.73105  H
H-HW-0.417000        0     1.14426  -6.21283   3.34853  H
H-HW-0.417000        0     1.72082  -4.29331   2.86503  H
O-OW--0.834000       0    -0.23286  -8.49593  -0.07205  L
H-HW-0.417000        0     0.00092  -7.59697  -0.34931  L
H-HW-0.417000        0    -0.50327  -8.90762  -0.91158  L
O-OW--0.834000       0     4.7428   -3.53461   4.24098  L
H-HW-0.417000        0     4.59825  -3.63191   3.27669  L
H-HW-0.417000        0     4.3268   -4.34392   4.60137  L
O-OW--0.834000       0     1.01058  -4.24376   5.31173  H
H-HW-0.417000        0     0.54415  -3.80792   4.58142  H
H-HW-0.417000        0     0.39676  -5.0268    5.37496  H
O-OW--0.834000       0    -0.98077  -9.33656  -2.6526   L
H-HW-0.417000        0    -0.71751  -8.43821  -2.91683  L
H-HW-0.417000        0    -0.89565  -9.78597  -3.53944  L
C-CW--0.220700       0     8.01307  -10.51327   10.46019  L
H-H4-0.186200        0     9.05194  -10.37588   10.18975  L
C-CT--0.149000       0     12.20678  -3.75814   12.93685  L
H-H1-0.097600        0     12.16906  -2.93545   13.65293  L
H-H1-0.097600        0     11.64893  -4.60834   13.32977  L
H-H1-0.097600        0     13.25032  -4.04616   12.79435  L
H-HC                 0    -6.92172  -10.14046  -7.55479  L
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