CARTESIAN COORDINATES (A.U.)

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NO LB ZA FRAG MASS X Y Z

0 C 6.0000 0 12.011 0.172050 -0.057185 0.262619

CARTESIAN COORDINATES (A.U.)

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NO LB ZA FRAG MASS X Y Z

0 C 6.0000 0 12.011 0.189044 -0.068550 0.287301

1 C 6.0000 0 12.011 -2.051547 -0.966064 1.559082

2 N 7.0000 0 14.007 2.043905 1.051446 1.372924

3 H 1.0000 0 1.008 -3.694490 -1.398330 0.424745

4 C 6.0000 0 12.011 -2.174799 -0.744450 4.076555

5 N 7.0000 0 14.007 2.371303 0.869200 3.954731

6 H 1.0000 0 1.008 -3.932924 -0.859908 5.111807

7 O 8.0000 0 15.999 2.208376 -1.723087 4.774291

8 C 6.0000 0 12.011 0.151157 -0.273827 5.439333

9 H 1.0000 0 1.008 0.085138 0.322454 7.397390

10 H 1.0000 0 1.008 0.179458 0.052992 -1.759678

INTERNAL COORDINATES (A.U.)

C 8 6 3 2.621254332124 63.04749227 250.87208549

H 9 8 6 2.049196904027 115.24998931 255.84170007

H 1 2 3 2.052202219505 118.61509285 191.37047621