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

1 C 6.0000 0 12.011 -2.065405 -0.931724 1.539921

2 N 7.0000 0 14.007 2.077733 1.010457 1.349208

3 H 1.0000 0 1.008 -3.731310 -1.326215 0.420585

4 C 6.0000 0 12.011 -2.160229 -0.776745 4.077201

5 N 7.0000 0 14.007 2.392429 0.882255 3.940202

6 H 1.0000 0 1.008 -3.908173 -0.972270 5.122320

7 O 8.0000 0 15.999 2.230533 -1.768324 4.879692

8 C 6.0000 0 12.011 0.156057 -0.272943 5.450471

9 H 1.0000 0 1.008 0.047149 0.409729 7.382695

10 H 1.0000 0 1.008 0.163786 0.064842 -1.786434