CARTESIAN COORDINATES (A.U.)

----------------------------

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

INTERNAL COORDINATES (A.U.)

---------------------------

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.720757479186 0.00000000 0.00000000

N 1 2 0 2.439705499957 125.02486672 0.00000000

H 2 1 3 2.045428090822 118.35030229 163.71456538

C 2 1 3 2.543777153216 118.64222546 355.94089564

N 3 1 2 2.613181925308 120.94350936 15.34111410

H 5 2 1 2.045925281111 122.38122717 165.15264023

O 6 3 1 2.816810631834 111.71199465 51.28666614

C 8 6 3 2.620191303466 65.23646425 252.93236692

H 9 8 6 2.052167456542 115.91113704 256.75752990

H 1 2 3 2.052699682386 118.97506710 192.37934276