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

CARTESIAN COORDINATES (A.U.)

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NO LB ZA FRAG MASS X Y Z

0 C 6.0000 0 12.011 0.183985 -0.044116 0.281663

1 C 6.0000 0 12.011 -2.083401 -0.922862 1.552402

2 N 7.0000 0 14.007 2.081954 0.991268 1.353738

3 H 1.0000 0 1.008 -3.729874 -1.353714 0.422600

4 C 6.0000 0 12.011 -2.173909 -0.760004 4.064974

5 N 7.0000 0 14.007 2.336848 0.841919 3.996921

6 H 1.0000 0 1.008 -3.904896 -0.976394 5.130368

7 O 8.0000 0 15.999 2.230616 -1.747238 4.830498

8 C 6.0000 0 12.011 0.176129 -0.226683 5.411848

9 H 1.0000 0 1.008 0.073913 0.396796 7.361216

10 H 1.0000 0 1.008 0.183257 0.062903 -1.767747

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

MULLIKEN ATOMIC CHARGES

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0 C : -0.052531

1 C : -0.141741

2 N : -0.115807

3 H : 0.148623

4 C : -0.146495

5 N : -0.018584

6 H : 0.161079

7 O : -0.236580

8 C : 0.113670

9 H : 0.138473

10 H : 0.149893

Sum of atomic charges: 0.0000000

LOEWDIN ATOMIC CHARGES

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0 C : -0.217884

1 C : -0.151142

2 N : 0.052992

3 H : 0.152129

4 C : -0.127445

5 N : 0.052008

6 H : 0.151234

7 O : 0.134240

8 C : -0.327692

9 H : 0.134794

10 H : 0.146766

LOEWDIN REDUCED ORBITAL CHARGES

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0 C s : 2.794859 s : 2.794859

pz : 1.001053 p : 2.861073

px : 0.989692

py : 0.870327

dz2 : 0.154713 d : 0.499446

dxz : 0.099614

dyz : 0.035212

dx2y2 : 0.094817

dxy : 0.115090

f0 : 0.004975 f : 0.062506

f+1 : 0.017235

f-1 : 0.004661

f+2 : 0.009417

f-2 : 0.009972

f+3 : 0.007173

f-3 : 0.009074

1 C s : 2.775877 s : 2.775877

pz : 1.071634 p : 2.960356

px : 0.994561

py : 0.894162

dz2 : 0.088285 d : 0.371626

dxz : 0.153835

dyz : 0.060210

dx2y2 : 0.035714

dxy : 0.033581

f0 : 0.007945 f : 0.043283

f+1 : 0.014116

f-1 : 0.007332

f+2 : 0.003732

f-2 : 0.002928

f+3 : 0.003734

f-3 : 0.003496

2 N s : 3.112783 s : 3.112783

pz : 1.079706 p : 3.548396

px : 1.284068

py : 1.184622

dz2 : 0.095137 d : 0.261961

dxz : 0.075205

dyz : 0.041992

dx2y2 : 0.023664

dxy : 0.025964

f0 : 0.006204 f : 0.023869

f+1 : 0.006998

f-1 : 0.004137

f+2 : 0.001457

f-2 : 0.001865

f+3 : 0.001514

f-3 : 0.001695

3 H s : 0.788881 s : 0.788881

pz : 0.017461 p : 0.058990

px : 0.028130

py : 0.013399

4 C s : 2.782159 s : 2.782159

pz : 1.075106 p : 2.930334

px : 1.000557

py : 0.854671

dz2 : 0.088045 d : 0.371618

dxz : 0.160072

dyz : 0.057358

dx2y2 : 0.035001

dxy : 0.031142

f0 : 0.007952 f : 0.043334

f+1 : 0.014209

f-1 : 0.006757

f+2 : 0.004196

f-2 : 0.002829

f+3 : 0.003795

f-3 : 0.003596

5 N s : 3.211579 s : 3.211579

pz : 1.103365 p : 3.374251

px : 1.259339

py : 1.011547

dz2 : 0.090013 d : 0.329891

dxz : 0.068480

dyz : 0.084016

dx2y2 : 0.049644

dxy : 0.037738

f0 : 0.007695 f : 0.032270

f+1 : 0.004809

f-1 : 0.007156

f+2 : 0.003677

f-2 : 0.002243

f+3 : 0.002934

f-3 : 0.003757

6 H s : 0.789466 s : 0.789466

pz : 0.016722 p : 0.059300

px : 0.029965

py : 0.012613

7 O s : 3.439259 s : 3.439259

pz : 1.607455 p : 4.314185

px : 1.439362

py : 1.267369

dz2 : 0.014499 d : 0.104532

dxz : 0.012513

dyz : 0.017249

dx2y2 : 0.028916

dxy : 0.031356

f0 : 0.000705 f : 0.007784

f+1 : 0.000482

f-1 : 0.001048

f+2 : 0.000948

f-2 : 0.000910

f+3 : 0.002178

f-3 : 0.001513

8 C s : 2.783349 s : 2.783349

pz : 0.988393 p : 2.778814

px : 0.924589

py : 0.865832

dz2 : 0.133378 d : 0.665076

dxz : 0.141274

dyz : 0.083549

dx2y2 : 0.128161

dxy : 0.178714

f0 : 0.009306 f : 0.100453

f+1 : 0.016486

f-1 : 0.005925

f+2 : 0.009426

f-2 : 0.020594

f+3 : 0.020540

f-3 : 0.018176

9 H s : 0.806527 s : 0.806527

pz : 0.036705 p : 0.058679

px : 0.008228

py : 0.013746

10 H s : 0.796024 s : 0.796024

pz : 0.037336 p : 0.057211

px : 0.009107

py : 0.010768