INTERNAL COORDINATES (ANGSTROEM)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.439762847297 0.00000000 0.00000000

N 1 2 0 1.291036545542 125.02486672 0.00000000

H 2 1 3 1.082393926880 118.35030229 163.71456538

C 2 1 3 1.346108892476 118.64222546 355.94089564

N 3 1 2 1.382836316015 120.94350936 15.34111410

H 5 2 1 1.082657028649 122.38122717 165.15264023

O 6 3 1 1.490591986463 111.71199465 51.28666614

C 8 6 3 1.386545519180 65.23646425 252.93236692

H 9 8 6 1.085960245617 115.91113704 256.75752990

H 1 2 3 1.086241887403 118.97506710 192.37934276

INTERNAL COORDINATES (ANGSTROEM)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.451915023386 0.00000000 0.00000000

N 1 2 0 1.277023455530 125.56358617 0.00000000

H 2 1 3 1.080993887006 118.52004292 165.63235662

C 2 1 3 1.333246434831 118.09018467 356.57609514

N 3 1 2 1.407421523032 119.52368467 14.37894899

H 5 2 1 1.081672822747 122.91296117 166.21212169

O 6 3 1 1.440477441288 110.73224819 54.10031780

C 8 6 3 1.387108049718 63.04749227 250.87208549

H 9 8 6 1.084388296930 115.24998931 255.84170007

H 1 2 3 1.085978641385 118.61509285 191.37047621

INTERNAL COORDINATES (ANGSTROEM)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.443713767868 0.00000000 0.00000000

N 1 2 0 1.282474541976 124.87399349 0.00000000

H 2 1 3 1.080977949413 118.11758911 163.18004685

C 2 1 3 1.338930658151 118.35947405 356.34954831

N 3 1 2 1.380547649132 120.46902327 18.34696121

H 5 2 1 1.081398133889 122.75207353 162.11500251

O 6 3 1 1.441284253010 110.90182642 48.66923269

C 8 6 3 1.377364174283 66.05972119 252.30329827

H 9 8 6 1.083702336791 115.58809120 256.83355703

H 1 2 3 1.085134430684 118.75023782 193.84947625

INTERNAL COORDINATES (ANGSTROEM)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.446089567928 0.00000000 0.00000000

N 1 2 0 1.282079682522 125.11937627 0.00000000

H 2 1 3 1.081135178305 118.25995985 164.02638319

C 2 1 3 1.338101186332 118.29239086 356.42201719

N 3 1 2 1.389747560366 120.16788827 16.87535393

H 5 2 1 1.081709011415 122.79461205 163.59936097

O 6 3 1 1.451862492244 110.93374572 50.51639318

C 8 6 3 1.382114614006 64.76229197 251.86768550

H 9 8 6 1.084345824121 115.46832024 256.36176048

H 1 2 3 1.085522251028 118.71471743 192.94958814

INTERNAL COORDINATES (ANGSTROEM)

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C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.447646478828 0.00000000 0.00000000

N 1 2 0 1.280783857725 125.21878343 0.00000000

H 2 1 3 1.081104841789 118.32731014 164.27343032

C 2 1 3 1.336868672677 118.22152207 356.45449671

N 3 1 2 1.394472474523 119.96476367 16.51223208

H 5 2 1 1.081689467440 122.84109695 164.00825542

O 6 3 1 1.447576707881 110.84670737 51.18921117

C 8 6 3 1.383434131979 64.32826787 251.58320313

H 9 8 6 1.084294007917 115.40666989 256.20978474

H 1 2 3 1.085564158230 118.66685014 192.70335062

INTERNAL COORDINATES (ANGSTROEM)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.447258568288 0.00000000 0.00000000

N 1 2 0 1.280992117689 125.18693205 0.00000000

H 2 1 3 1.081091385480 118.30500075 164.19973281

C 2 1 3 1.337068523958 118.23831950 356.45249306

N 3 1 2 1.392955240922 120.03208445 16.64379836

H 5 2 1 1.081668690909 122.83131479 163.87811064

O 6 3 1 1.447835626603 110.85201310 50.96352983

C 8 6 3 1.382813139084 64.49005345 251.66647136

H 9 8 6 1.084265747090 115.42388340 256.26038135

H 1 2 3 1.085539183009 118.68059740 192.79173885

INTERNAL COORDINATES (ANGSTROEM)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 1.447303092309 0.00000000 0.00000000

N 1 2 0 1.280967044569 125.19018758 0.00000000

H 2 1 3 1.081090443926 118.30741343 164.22048519

C 2 1 3 1.337038981509 118.23615765 356.46086984

N 3 1 2 1.393050901801 120.02999291 16.61912574

H 5 2 1 1.081668228615 122.83236168 163.90024428

O 6 3 1 1.447877532703 110.85096421 50.98858035

C 8 6 3 1.382849786124 64.47480668 251.66123360

H 9 8 6 1.084268843109 115.42161286 256.25327379

H 1 2 3 1.085543496690 118.68056751 192.77715784

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

INTERNAL COORDINATES (A.U.)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.743721763925 0.00000000 0.00000000

N 1 2 0 2.413224597545 125.56358617 0.00000000

H 2 1 3 2.042782398885 118.52004292 165.63235662

C 2 1 3 2.519470630857 118.09018467 356.57609514

N 3 1 2 2.659641233517 119.52368467 14.37894899

H 5 2 1 2.044065401498 122.91296117 166.21212169

O 6 3 1 2.722107866127 110.73224819 54.10031780

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

INTERNAL COORDINATES (A.U.)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.728223637043 0.00000000 0.00000000

N 1 2 0 2.423525658061 124.87399349 0.00000000

H 2 1 3 2.042752281198 118.11758911 163.18004685

C 2 1 3 2.530212256216 118.35947405 356.34954831

N 3 1 2 2.608856971689 120.46902327 18.34696121

H 5 2 1 2.043546314783 122.75207353 162.11500251

O 6 3 1 2.723632519322 110.90182642 48.66923269

C 8 6 3 2.602841076069 66.05972119 252.30329827

H 9 8 6 2.047900627225 115.58809120 256.83355703

H 1 2 3 2.050606892480 118.75023782 193.84947625

INTERNAL COORDINATES (A.U.)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.732713248505 0.00000000 0.00000000

N 1 2 0 2.422779481831 125.11937627 0.00000000

H 2 1 3 2.043049400745 118.25995985 164.02638319

C 2 1 3 2.528644781643 118.29239086 356.42201719

N 3 1 2 2.626242284376 120.16788827 16.87535393

H 5 2 1 2.044133788169 122.79461205 163.59936097

O 6 3 1 2.743622494454 110.93374572 50.51639318

C 8 6 3 2.611818106162 64.76229197 251.86768550

H 9 8 6 2.049116642049 115.46832024 256.36176048

H 1 2 3 2.051339766722 118.71471743 192.94958814

INTERNAL COORDINATES (A.U.)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.735655383720 0.00000000 0.00000000

N 1 2 0 2.420330727847 125.21878343 0.00000000

H 2 1 3 2.042992073038 118.32731014 164.27343032

C 2 1 3 2.526315668378 118.22152207 356.45449671

N 3 1 2 2.635171078140 119.96476367 16.51223208

H 5 2 1 2.044096855409 122.84109695 164.00825542

O 6 3 1 2.735523535738 110.84670737 51.18921117

C 8 6 3 2.614311633760 64.32826787 251.58320313

H 9 8 6 2.049018723614 115.40666989 256.20978474

H 1 2 3 2.051418959856 118.66685014 192.70335062

INTERNAL COORDINATES (A.U.)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.734922339035 0.00000000 0.00000000

N 1 2 0 2.420724282145 125.18693205 0.00000000

H 2 1 3 2.042966644299 118.30500075 164.19973281

C 2 1 3 2.526693332567 118.23831950 356.45249306

N 3 1 2 2.632303922153 120.03208445 16.64379836

H 5 2 1 2.044057593455 122.83131479 163.87811064

O 6 3 1 2.736012821214 110.85201310 50.96352983

C 8 6 3 2.613138127256 64.49005345 251.66647136

H 9 8 6 2.048965318392 115.42388340 256.26038135

H 1 2 3 2.051371763527 118.68059740 192.79173885

INTERNAL COORDINATES (A.U.)

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

C 0 0 0 0.000000000000 0.00000000 0.00000000

C 1 0 0 2.735006477242 0.00000000 0.00000000

N 1 2 0 2.420676900814 125.19018758 0.00000000

H 2 1 3 2.042964865019 118.30741343 164.22048519

C 2 1 3 2.526637505428 118.23615765 356.46086984

N 3 1 2 2.632484695015 120.02999291 16.61912574

H 5 2 1 2.044056719846 122.83236168 163.90024428

O 6 3 1 2.736092012266 110.85096421 50.98858035

C 8 6 3 2.613207380126 64.47480668 251.66123360

H 9 8 6 2.048971169020 115.42161286 256.25327379

H 1 2 3 2.051379915204 118.68056751 192.77715784