Au

1.00000000000000

0.0000000000000000 2.0486125629534273 2.0486125629534273

2.0486125629534273 -0.0000000000000000 2.0486125629534273

2.0486125629534273 2.0486125629534273 -0.0000000000000000

Au

1

Direct

0.5012285012285034 0.5012285012285034 0.5012285012285034

0.00000000E+00 0.00000000E+00 0.00000000E+00