

3irfe

P LATTICE,NONEQUIV.ATOMS: 2

MODE OF CALC=RELA unit=bohr

7.22596 7.22596 7.22596 90.00000 90.00000 90.00000  
ATOM 1: X=0.00000000 Y=0.00000000 Z=0.00000000MULT= 1 ISPLIT= 2  
Fe NPT= 781 R0=0.00005000 RMT= 2.4600 Z: 26.0  
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000  
0.0000000 1.0000000 0.0000000  
0.0000000 0.0000000 1.0000000

ATOM -2: X=0.50000000 Y=0.50000000 Z=0.00000000

MULT= 3 ISPLIT=-2  
-2: X=0.50000000 Y=0.00000000 Z=0.50000000  
-2: X=0.00000000 Y=0.50000000 Z=0.50000000Ir NPT= 781 R0=0.00005000 RMT= 2.4600 Z: 77.0  
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000  
0.0000000 1.0000000 0.0000000  
0.0000000 0.0000000 1.0000000