

.m40

	10	0	0	1	0				
	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	100000
	0.000000	0.000000	0.000000						000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	000000
Fe	1	1	0.500000	0.127000	-0.250000	0.750000			000 0 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0101100000
01	3	1	1.000000	0.125000	-0.253000	0.433000			000 0 0 0
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
02	3	1	0.500000	0.288000	-0.017000	0.250000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
τ	0.500000								0
	0.000000	0.000000							00
	0.000000								0
02a	3	1	0.500000	0.288000	0.517000	0.250000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
$1 - \tau$	0.500000								0
	0.500000	0.000000							00
	0.000000								0
03	3	1	0.500000	-0.042000	-0.018000	0.250000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
τ	0.500000								0
	0.000000	0.000000							00
	0.000000								0
03a	3	1	0.500000	-0.042000	0.518000	0.250000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
$1 - \tau$	0.500000								0
	0.500000	0.000000							00
	0.000000								0
Se	2	1	0.500000	0.124000	0.867000	0.250000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
τ	0.500000								0
	0.000000	0.000000							00
	0.000000								0
Sea	2	1	0.500000	0.124000	0.633000	0.250000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
$1 - \tau$	0.500000								0
	0.500000	0.000000							00
	0.000000								0
04	3	1	0.500000	-0.126000	-0.341000	0.750000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
τ	0.500000								0
	0.000000	0.000000							00
	0.000000								0
04a	3	1	0.500000	-0.126000	0.841000	0.750000			100 1 0 0
	0.030000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0000000000
$1 - \tau$	0.500000								0
	0.500000	0.000000							00
	0.000000								0

.m50

```

Version Jana2006
title
cell 7.589 7.259 6.562 90 90 90
esdcell 0.03 0.04 0.04 0 0 0
ndim 4 ncomp 1
qi 0 0 0.5
qr 0 0 0
spgroup Pnam(00g)000 62 3
lattice P
symmetry x1 x2 x3 x4
symmetry -x1 -x2 x3+1/2 x4
symmetry -x1+1/2 x2+1/2 -x3 -x4
symmetry x1+1/2 -x2+1/2 -x3+1/2 -x4
symmetry -x1 -x2 -x3 -x4
symmetry x1 x2 -x3+1/2 -x4
symmetry x1+1/2 -x2+1/2 x3 x4
symmetry -x1+1/2 x2+1/2 x3+1/2 x4
unitsnumb 4
atlist Fe S 05 H0
formtab -62
atom Fe atradius 1.26 color 181113000
atom S atradius 1.04 color 255250000
atom O atradius 0.74 color 254003000
atom H atradius 0.46 color 255204204
comen 1 0 -2
comen 0 1 0
comen 1 0 0
tzero 0
lambda 0.71075 radtype 1 lpfactor 1
monangle 6.0823 perfmono 0.5
nalpha 2 kalpha1 0.709317 kalpha2 0.713607 kalphar 0.499
roundmethod 1
end

```

$\mathbf{q} = \gamma \mathbf{c}^* = \frac{1}{2} \mathbf{c}^*$

to