chksymbreak 0

ndtset 28

ecut: 6

ecut+ 2

occopt 4 #Cold smearing of N Mazari

tsmear 0.0005

acell 2\*5.144312078066 44.91895577

angdeg 90 90 120

paral\_kgb 1 npfft 4 npband 24 npkpt 4 bandpp 2

max\_ncpus 48

ntypat 1

znucl 46

typat 3\*1

xred

0.0 0.0 0.0 # Triplet giving the REDUCED coordinate of atom 1.

1/3 2/3 1/10

2/3 1/3 2/10

ixc 11 # GGA Perdew-Burke-Ernzerhof GGA functional

ngkpt 4 4 1

shiftk 0 0 0

nstep 480

tolvrs 1.0d-12

iprcel 45

iscf 7

npulayit 30

diemac 1e+8

diemix 1

nnsclo 3

timopt -3

nband 48

ngfft 64 64 160

nline 6 #commented out while it improves precision and convergence?, it slows the calculation greatly.

optforces 0

nbdbuf 6