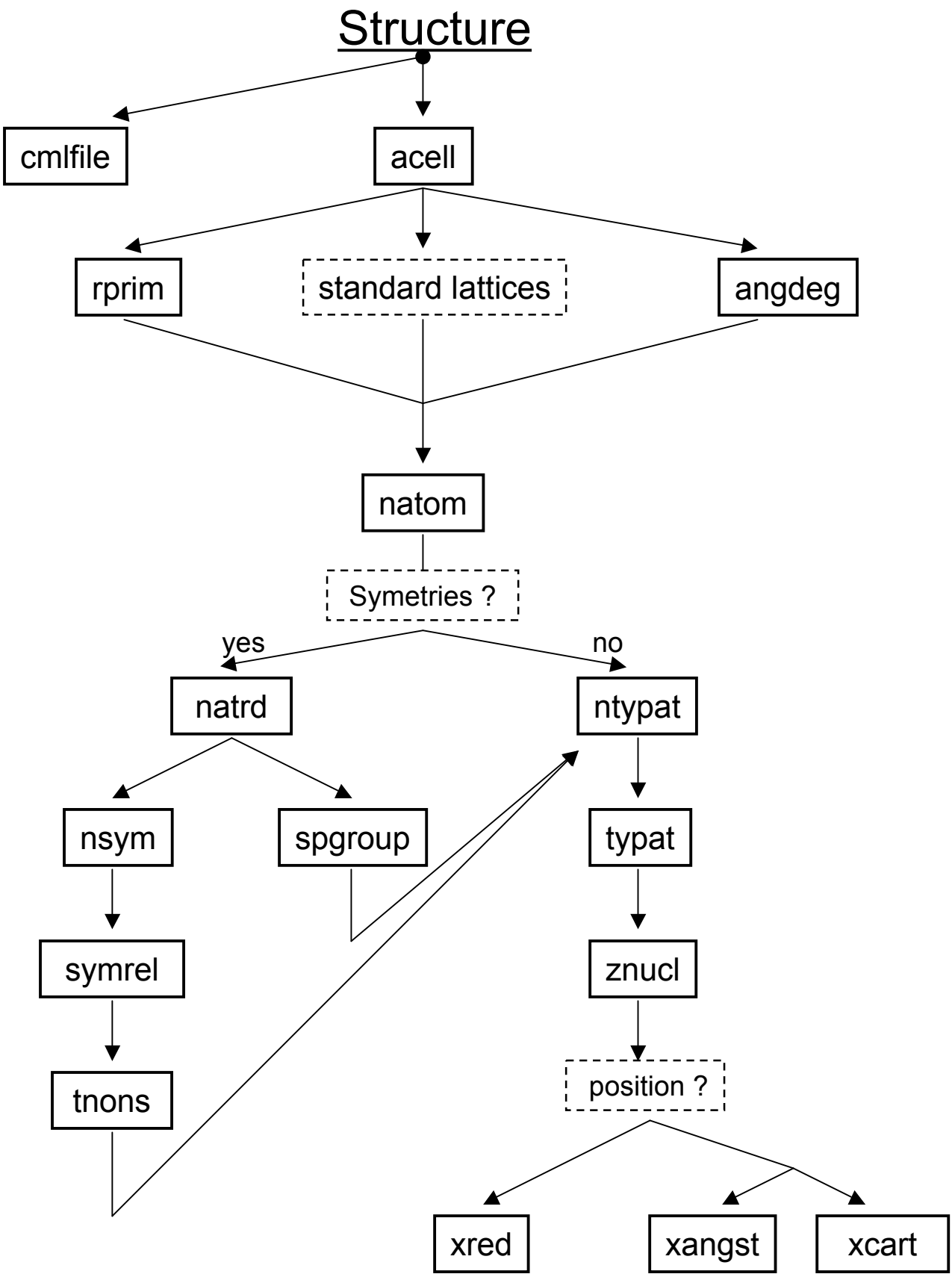
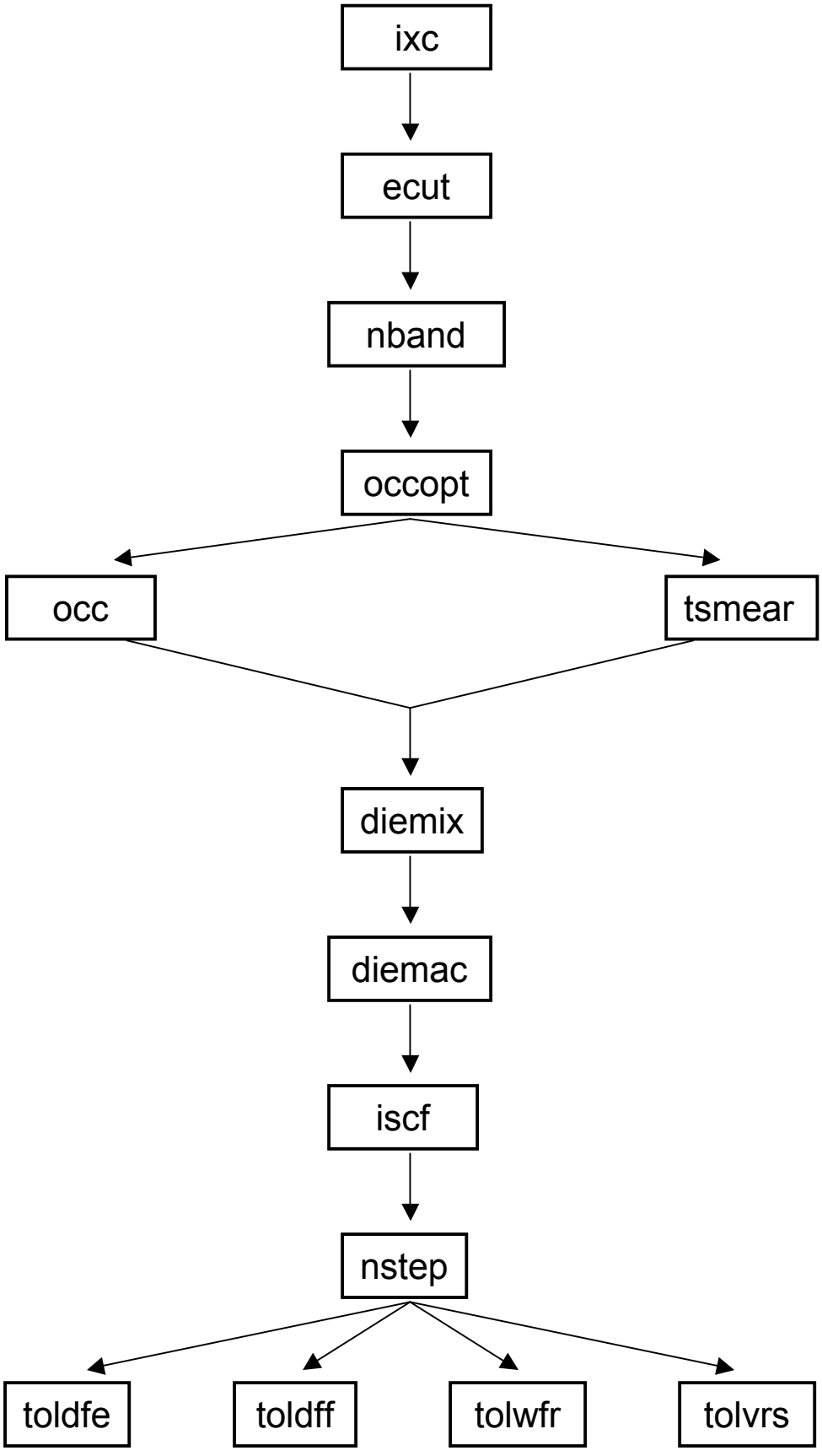
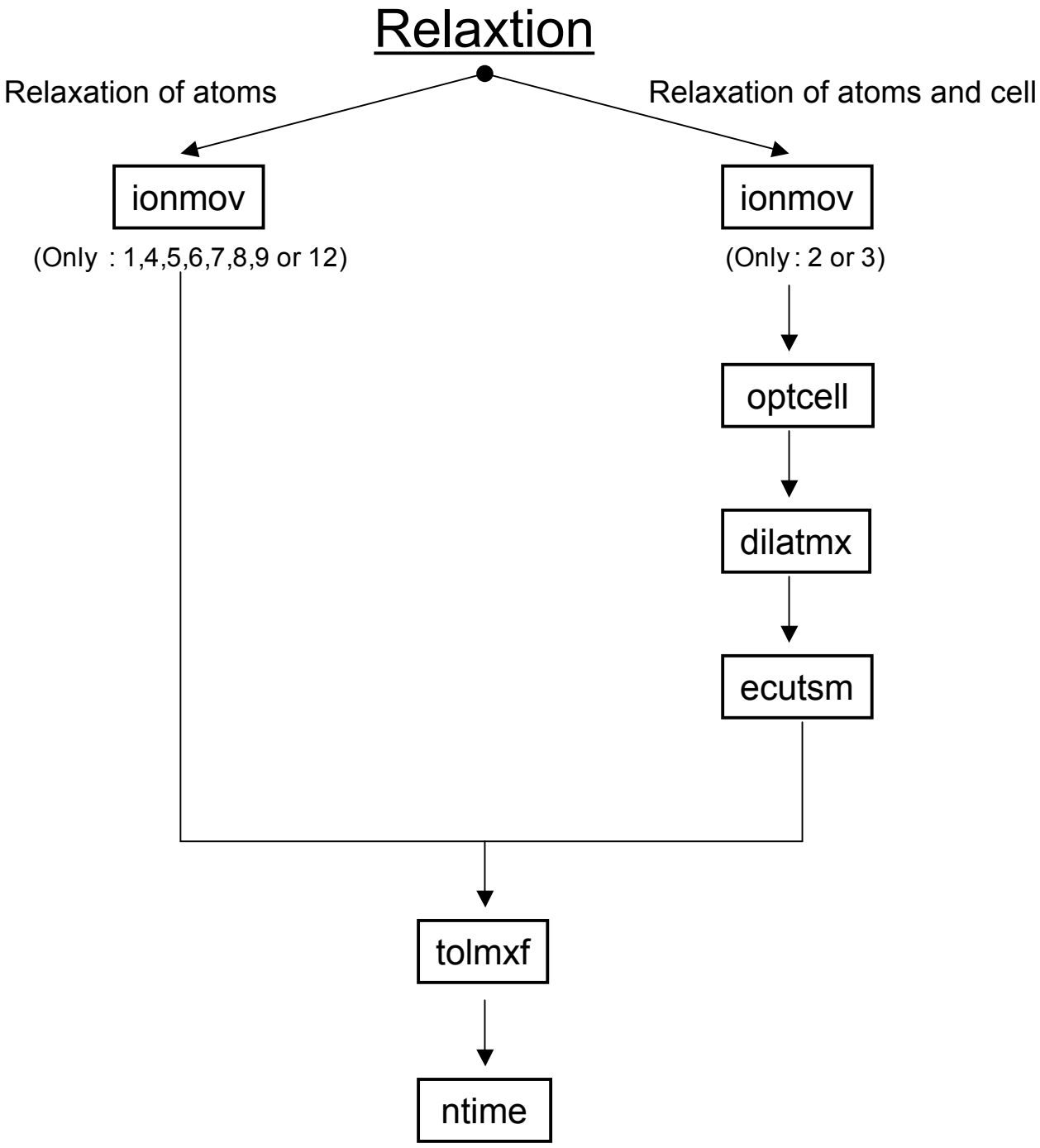
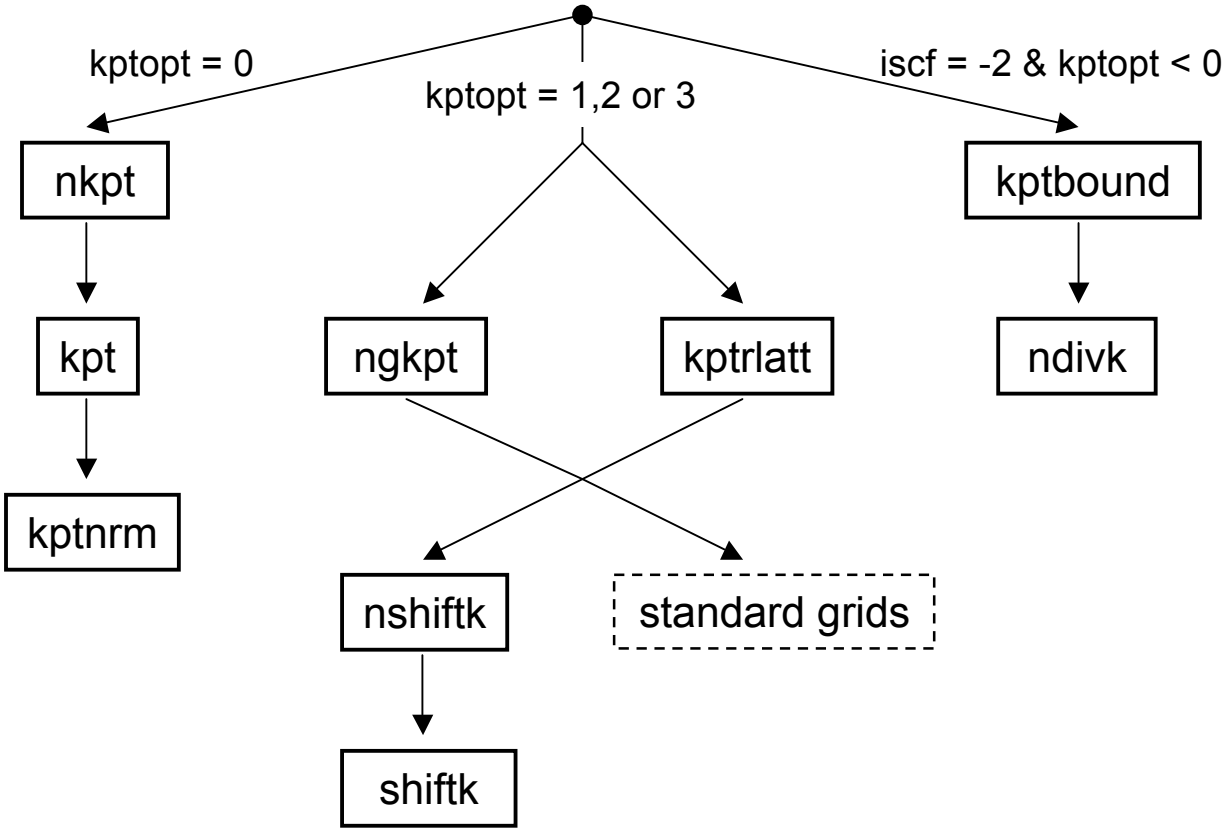

Structure
cmlfile
acell
rprim
standard lattices
angdeg
natom
Symetries ?
yes
no
natrd
ntypat
nsym
spgroup
typat
symrel
znucl
tnons
position ?
xred
xangst
xcart

Calculation Parameter




Relaxtion
Relaxation of atoms
Relaxation of atoms and cell
ionmov
(Only : 1,4,5,6,7,8,9 or 12)
ionmov
(Only : 2 or 3)
optcell
dilatmx
ecutsm
tolmxf
ntime

K-points Grid