

```
%chk=test
%mem=100MB
%nproc=1
# opt=(calcall,ts, maxcycle=100, noeigentest) freq=readiso ub3lyp/6-31g
scf=qc scfcyc=200 geom=
Allcheck guess=(Tcheck, nosymm)
```

```
298.15 1
12
1
2
12
1
2
```