

File format for Norm-Conserving Pseudopotentials

The pseudopotential files consist of a number of header lines, followed by the data on a radial grid. The three first lines of the header have the same format and meaning for all norm-conserving pseudopotential files that can be read by ABINIT. They are :

```
title (single 80 character line)
zatom, zion, pspdat
pspcod, pspxc, lmax, lloc, mmax, r2well
```

The data may be located anywhere on the line as long as it is provided in the order indicated (it is read with free format). In the case of Si with $l_{\max}=2$, the header may look like the following 10 lines:

```
Si Fri Oct 08 11:18:59 1993
14.00000 4.00000 930920 zatom, zion, pspdat
1 1 2 2 2001 .00050
pspcod, pspxc, lmax, lloc, mmax, r2well
```

The first line is free, and might contain information useful for the pseudopotential generator only. In the present case, it means that this silicon pseudopotential was created in 1993. The next two lines are important for ABINIT, with the following meaning:

```
zatom : atomic number of the atom (14 for Si)
zion : number of valence electrons (4 for Si)
pspcod : code revision date (930920 for this case)
pspxc : identifier for the pseudopotential format
pspxc : the choice of exchange-correlation, coherent with the ABINIT
nomenclature
lmax : highest angular momentum for which a pseudopotential
is defined, which is also used for the local potential
lloc : angular momentum used for the local potential
mmax : number of grid points
r2well : prefactor of a harmonic well sometimes used to bind
electrons which would otherwise be unbound in lda (usually 0.000)
```

At this point, differences might appear in the different file formats, that are described in the following pages:

- [psp1_format](#)
- [psp3_format](#)
- [psp45_format](#)
- [psp5_spinorbit_format](#)
- [psp6_format](#)
- [psp8_format](#)

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