# OptaDOS: User Guide

Version 0.9

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# Chapter 1

# Parameters

## 1.1 Usage

```
optados.x [seedname]
```

- `seedname`: If a seedname string is given the code will read its input from a file `seedname.odi`. The default value is `castep`.

## 1.2 `seedname.odi` File

The `OptaDOS` input file `seedname.odi` has a flexible free-form structure.

The ordering of the keywords is not significant. Case is ignored (so `smearing_width` is the same as `Smearing_Width`). Characters after !, or # are treated as comments. Most keywords have a default value that is used unless the keyword is given in `seedname.odi`. Keywords can be set in any of the following ways

```
smearing_width = 0.4
smearing_width :  0.4
smearing_width 0.4
```

A logical keyword can be set to `.true.` using any of the following strings: `T`, `true`, `.true.`.

## 1.3 Parameters

### 1.3.1 `character(len=50) :: task`

Tells the code what to compute.

The valid options for this parameter are:

- `dos` (default)
- `jdos`
- `pdos`
- `optics`
- `core`
- `all`

### 1.3.2 `character(len=50) :: spectral_scheme`

Which method to use compute dos etc

The valid options for this parameter are:

- `adaptive` (default)
- `fixed`
- `linear`
- `quad`

### 1.3.3 `integer :: iprint`

This indicates the level of verbosity of the output from 0, the bare minimum, to 3, which corresponds to full debugging output.

The default value is 1.

### 1.3.4 `character(len=20) :: energy_unit`

The energy unit to be used for writing quantities in the output files.

The valid options for this parameter are:

- `eV` (default)

- Ry
- Ha

### 1.3.5 real(kind=dp) :: adaptive_smearing

Set the relative smearing in the adaptive scheme

Default value is 0.4

### 1.3.6 real(kind=dp) :: smearing_width

Smearing width for broadening

If spectral_scheme = fixed default value is 0.5eV, else default value is 0.0eV

### 1.3.7 real(kind=dp) :: scissor_op

Value of the scissor operator.

Default value is 0eV

### 1.3.8 logical :: compute_efermi

If compute_efermi=TRUE, then OptaDOS will use the value of the fermi level computed from the integration of the DOS. If compute_efermi=FALSE, then the value set by fermi_energy will be used, if fermi_energy is not set the value from the bands file will be used.

The default value is FALSE.

### 1.3.9 real(kind=dp) :: fermi_energy

Value of the fermi energy

No default value

### 1.3.10 character(len=20) :: output_format

Format in which to output data

The valid options for this parameter are:

- gnuplot (default)
- grace

### 1.3.11 `integer :: pdos`

Defines which components to include in the pdos analysis:

- `angular` (decompose as s,p,d etc)
- `atom` (decompose onto atomic sites)
- `C:H` (decompose onto Carbon and Hydrogen sites)
- `C1:C3:C4-C8` (decompose onto atoms C1, C2 and C4,C5,C6,C7,C8)
- `Si1[s;d]` (decompose onto 's' and 'd' channels for atom Si1)

### 1.3.12 `character(len=50) :: devel_flag`

Not a regular keyword. Its purpose is to allow a developer to pass a string into the code to be used inside a new routine as it is developed.

No default.