ecx

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NAME

ecx - library for electrochemistry

SYNOPSIS

```
ecx (Fortran): use ecx
ecx (C): include "ecx.h"
ecx (python): import pyecx
```

DESCRIPTION

ecx a Fortran library for providing a collection of routines for electrochemistry. A C API allows usage from C, or can be used as a basis for other wrappers. A Python wrapper allows easy usage from Python.

It covers:

o kinetics
Nernst, Butler-Volmer

o electrochemical
Impedance, Admittance, Circuit Elements, Equivalent Circuits

o photoelectrochemistry
Photocurrent, Band-gap, space charge.

The C API is defined by adding a prefix to the functions from the Fortran API due to the lack of module/namespace feature in the C language. The functions are therefore following this template: (c_prefix)fortran_func.

- (ecx_)get_version
- (ecx_core_)kTe
- (ecx_eis_)z
- mm
- (ecx_kinetics_)nernst
- (ecx_kinetics_)sbv
- (ecx_kinetics_)bv
- (ecx_eis_)z

NOTES

To use ecx within your fpm <https://github.com/fortran-lang/fpm> project, add the following lines to your file:

```
[dependencies]
ecx = { git="https://github.com/MilanSkocic/ecx.git" }
```

EXAMPLE

Minimal example in Fortran:

```
use ecx
```

Minimal example in C:

```
include "ecx.h"
```

Minimal example in Python:

```
import pyecx
```

SEE ALSO

complex(7), **gsl**(3), **catanh**(3), **gnuplot**(1), **ecx_get_version**(3)

NAME

ecxcli(1) - Command line for ecx

SYNOPSIS

ecxcli *SUBCOMMAND* [*OPTIONS* ...] *ARGS* ...

DESCRIPTION

ecxcli is command line interface for computing electro- chemical properties:

- **EIS** Electrochemical Impedance **Z=f**(w)
- **Kinetics**
  j=f(U)
- **PEC** **Iph=f**(hv, U)

It can also provide the molar masses, isotope compositions and nuclide compositions.

SUBCOMMANDS

- **all** Get the whole periodic table.
- **saw** Get the standard atomic weight.

Enter **ecxcli** *SUBCOMMAND* **--help** for detailed descriptions.

OPTIONS

- **--abridged, -a**
  Use the abridged value.
- **--uncertainty, -u**
  Use the uncertainty.
- **--pprint**
  Nice formatting.
- **--mass, -z**
  Get the mass number.

VALID FOR ALL SUBCOMMANDS

- **--help**
  Show help text and exit
- **--verbose**
  Display additional information when available.
- **--version**
  Show version information and exit.

NAME

get_version - version getter for the library

LIBRARY

Electrochemistry library - (**-libecx**, **-lecx**)

SYNOPSIS

```
get_version()
```

DESCRIPTION

This function returns the version of the ecx library.

RETURN VALUE

character(len=:), pointer :: fptr

NAME

kTe - thermal voltage

LIBRARY

Electrochemistry library - (**-libecx**, **-lecx**)

SYNOPSIS

`kTe` (*`T`*)

DESCRIPTION

Compute the thermal voltage.

Parameters:

o *T* Temperature in degC

RETURN VALUE

real(dp) :: r

Thermal voltage in Volts.