

ecx

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NAME

ecx - library for electrochemistry

SYNOPSIS

```
use ecx
```

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

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)

NAME

ecxcli(1) - Command line for ecx

SYNOPSIS

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

DESCRIPTION

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

- o **EIS** Electrochemical Impedance $Z=f(w)$
- o **Kinetics**
 $j=f(U)$
- o **PEC** $I_{ph}=f(hv, U)$

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

SUBCOMMANDS

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

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

OPTIONS

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

VALID FOR ALL SUBCOMMANDS

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

SYNOPSIS

kTe (T)

DESCRIPTION

Compute the thermal voltage.

Parameters:

o T Temperature in ^\circ C

RETURN VALUE

real(dp) :: r

Thermal voltage in Volts.