

## **ecx**

*M. Skocic*

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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:

- 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

**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.