ciaaw Documentation

Release 0.1.0

M. Skocic

Dec 23, 2023

CONTENTS:

CHAPTER

ONE

GETTING STARTED

Sources: https://github.com/MilanSkocic/ciaaw

1.1 ciaaw

Modern Fortran
CIAAW

ciaaw is a Fortran library providing the standard and abreged atomic weights, the isotopic abundance and the isotopes standard atomic weights. It also provides a API for the C language. The formulas are taken from http://ciaaw.org.

1.1.1 How to install

A Makefile is provided, which uses fpm, for building the library.

On windows, msys2 needs to be installed. The MSVC compiler is only necessary for compiling the python wrapper. Add the msys2 binary (usually C:msys64usrbin) to the path in order to be able to use make.

On Darwin, the gcc toolchain needs to be installed.

Build: the configuration file will set all the environmental variables necessary for the compilation

```
chmod +x configure.sh
. ./configure.sh
make
```

Run tests

```
make test
```

Install

```
make install
```

Uninstall

```
make uninstall
```

If building the python wrapper is needed:

```
cd pywrapper
make clean
make plat=(windows, linux or darwin)
```

1.1.2 Dependencies

```
gcc>=10.0
gfortran>=10.0
fpm>=0.7
```

1.1.3 License

`GNU General Public License v3 (GPLv3)`

1.2 pyciaaw

Python wrapper around the Fortran ciaaw library. The Fortran library does not need to be installed, the python wrapper embeds all needed dependencies. On linux, you might have to install *libgfortran* if it is not distributed with your linux distribution.

1.2.1 How to install

```
pip install pyciaaw
```

1.2.2 Dependencies

```

```

1.2.3 License

`GNU General Public License v3 (GPLv3)`

1.3 Examples

1.3.1 Example in Fortran

```
program example_in_f
    use ciaaw
    implicit none

    print *, "version ", ciaaw_version_version

end program
```

1.3.2 Example in C

```c
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include "ciaaw.h"


int main(void){

    printf("version %s\n", ciaaw_version_capi_version);

    return EXIT_SUCCESS;
}
```

1.3.3 Example in Python

```python
r"""Example in python"""
import pyciaaw


print("version ", pyciaaw.__version__)
```

CHAPTER

TWO

CIAAW - THEORETICAL BACKGROUND

2.1 Standard Atomic Weights

The standard atomic weights (or realtive atomic mass), $A_r(E)$, are extracted from table 1 in Prohaska *et al.* [1]. For the elements that feature an interval for the standard atomic weight, the mean value and the uncertainty are computed using formulas defined in van der Veen *et al.* [2]:

$$A_r(E) = \frac{a+b}{2}$$
$$u(A_r(E)) = \frac{b-a}{2\sqrt{3}}$$

The standard atomic weights are a dimensionless quantity and thus they need to be multiplied by the molar mass constant $M_u = 0.99999999965 \pm 0.00000000030 g.mol^{-1}$ in order to get the value in $g.mol^{-1}$.

CHAPTER

THREE

RELEASE NOTES

3.1 iapws 0.1.0 Release Note

3.1.1 Changes

3.1.2 Download

iapws

pyiapws

3.1.3 Contributors

Milan Skocic

3.1.4 Commits

Full Changelog: https://github.com/MilanSkocic/ciaaw/compare/. . . .0.1.0

CHAPTER

FOUR

API

4.1 ciaaw

4.1.1 Fortran

- *iapws.f90*: Main module for the whole library.

```
module ciaaw
    use ciaaw__version
    use ciaaw__version_capi
    use ciaaw__saw
    use ciaaw__saw_capi
    implicit none

end module
```

SAW (Standard Atomic Weights)

- *ciaaw_saw.f90*: Module for Standard atomic weights

```
module ciaaw__saw
!! Standard Atomic Weights - autogenerated.
use iso_fortran_env
use ieee_arithmetic
implicit none
private

integer(int64), parameter :: x = 1
real(real64), parameter :: nan = transfer(huge(x), 1.0d0)

type, public :: ciaaw_saw_element_t
!! Object representing an element.
character(len=24) :: element !! Element name
character(len=8) :: symbol !! Element symbol
integer(int32) :: z !! Element atomic number
real(real64) :: saw_min !! Min standard atomic weight
real(real64) :: saw_max !! Max standard atomic weight
real(real64) :: saw !! Value standard atomic weight
real(real64) :: saw_u !! Uncertainty standard atomic weight
real(real64) :: asaw !! Abridged value standard atomic weight
real(real64) :: asaw_u !! Abridged uncertainty standard atomic weight
end type
```

(continues on next page)

(continued from previous page)

```
integer(int32), parameter, public :: ciaaw_saw_YEAR = 2021

type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_H =&
ciaaw_saw_element_t("hydrogen", "H", 1, &
1.00784d0, 1.00811d0, &
1.00798d0, 0.00008d0, &
1.0080d0, 0.0002d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_He =&
ciaaw_saw_element_t("helium", "He", 2, &
nan, nan, &
4.002602d0, 0.000002d0, &
4.0026d0, 0.0001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Li =&
ciaaw_saw_element_t("lithium", "Li", 3, &
6.938d0, 6.997d0, &
6.97d0, 0.02d0, &
6.94d0, 0.06d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Be =&
ciaaw_saw_element_t("beryllium", "Be", 4, &
nan, nan, &
9.0121831d0, 0.0000005d0, &
9.0122d0, 0.00001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_B =&
ciaaw_saw_element_t("boron", "B", 5, &
10.806d0, 10.821d0, &
10.813d0, 0.005d0, &
10.81d0, 0.02d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_C =&
ciaaw_saw_element_t("carbon", "C", 6, &
12.0096d0, 12.0116d0, &
12.0106d0, 0.0006d0, &
12.011d0, 0.002d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_N =&
ciaaw_saw_element_t("nitrogen", "N", 7, &
14.00643d0, 14.00728d0, &
14.0069d0, 0.0003d0, &
14.007d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_O =&
ciaaw_saw_element_t("oxygen", "O", 8, &
15.99903d0, 15.99977d0, &
15.9994d0, 0.0003d0, &
15.999d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_F =&
ciaaw_saw_element_t("fluorine", "F", 9, &
nan, nan, &
18.998403162d0, 0.000000005d0, &
18.998d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ne =&
ciaaw_saw_element_t("neon", "Ne", 10, &
nan, nan, &
20.1797d0, 0.0006d0, &
20.180d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Na =&
ciaaw_saw_element_t("sodium", "Na", 11, &
nan, nan, &
22.98976928d0, 0.00000002d0, &
```

(continues on next page)

(continued from previous page)

```
22.990d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Mg =&
ciaaw_saw_element_t("magnesium", "Mg", 12, &
24.304d0, 24.307d0, &
24.3055d0, 0.0009d0, &
24.305d0, 0.002d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Al =&
ciaaw_saw_element_t("aluminium", "Al", 13, &
nan, nan, &
26.9815384d0, 0.0000003d0, &
26.982d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Si =&
ciaaw_saw_element_t("silicon", "Si", 14, &
28.084d0, 28.086d0, &
28.0850d0, 0.0006d0, &
28.085d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_P =&
ciaaw_saw_element_t("phosphorous", "P", 15, &
nan, nan, &
30.973761998d0, 0.000000005d0, &
30.974d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_S =&
ciaaw_saw_element_t("sulfur", "S", 16, &
32.059d0, 32.076d0, &
32.067d0, 0.005d0, &
32.06d0, 0.02d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Cl =&
ciaaw_saw_element_t("chlorine", "Cl", 17, &
35.446d0, 35.457d0, &
35.451d0, 0.004d0, &
35.45d0, 0.01d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ar =&
ciaaw_saw_element_t("argon", "Ar", 18, &
39.792d0, 39.963d0, &
39.88d0, 0.05d0, &
39.95d0, 0.16d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_K =&
ciaaw_saw_element_t("potassium", "K", 19, &
nan, nan, &
39.0983d0, 0.0001d0, &
39.098d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ca =&
ciaaw_saw_element_t("calcium", "Ca", 20, &
nan, nan, &
40.078d0, 0.004d0, &
40.078d0, 0.004d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Sc =&
ciaaw_saw_element_t("scandium", "Sc", 21, &
nan, nan, &
44.955907d0, 0.000004d0, &
44.956d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ti =&
ciaaw_saw_element_t("titanium", "Ti", 22, &
nan, nan, &
47.867d0, 0.001d0, &
47.867d0, 0.001d0)
```

(continues on next page)

(continued from previous page)

```
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_V =&
ciaaw_saw_element_t("vanadium", "V", 23, &
nan, nan, &
50.9415d0, 0.0001d0, &
50.942d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Cr =&
ciaaw_saw_element_t("chromium", "Cr", 24, &
nan, nan, &
51.9961d0, 0.0006d0, &
51.996d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Mn =&
ciaaw_saw_element_t("manganese", "Mn", 25, &
nan, nan, &
54.938043d0, 0.000002d0, &
54.938d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Fe =&
ciaaw_saw_element_t("iron", "Fe", 26, &
nan, nan, &
55.845d0, 0.002d0, &
55.845d0, 0.002d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Co =&
ciaaw_saw_element_t("cobalt", "Co", 27, &
nan, nan, &
58.933194d0, 0.000003d0, &
58.933d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ni =&
ciaaw_saw_element_t("nickel", "Ni", 28, &
nan, nan, &
58.6934d0, 0.0004d0, &
58.693d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Cu =&
ciaaw_saw_element_t("copper", "Cu", 29, &
nan, nan, &
63.546d0, 0.003d0, &
63.546d0, 0.003d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Zn =&
ciaaw_saw_element_t("zinc", "Zn", 30, &
nan, nan, &
65.38d0, 0.02d0, &
65.38d0, 0.02d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ga =&
ciaaw_saw_element_t("gallium", "Ga", 31, &
nan, nan, &
69.723d0, 0.001d0, &
69.723d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Ge =&
ciaaw_saw_element_t("germanium", "Ge", 32, &
nan, nan, &
72.630d0, 0.008d0, &
72.630d0, 0.008d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_As =&
ciaaw_saw_element_t("arsenic", "As", 33, &
nan, nan, &
74.921595d0, 0.000006d0, &
74.922d0, 0.001d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Se =&
```

(continues on next page)

(continued from previous page)

```
ciaaw_saw_element_t("selenium", "Se", 34, &
nan, nan, &
78.971d0, 0.008d0, &
78.971d0, 0.008d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Br =&
ciaaw_saw_element_t("bromine", "Br", 35, &
79.901d0, 79.907d0, &
79.904d0, 0.002d0, &
79.904d0, 0.003d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Kr =&
ciaaw_saw_element_t("krypton", "Kr", 36, &
nan, nan, &
83.798d0, 0.002d0, &
83.798d0, 0.002d0)
type(ciaaw_saw_element_t), parameter, public :: ciaaw_saw_Tc =&
ciaaw_saw_element_t("technetium", "Tc", 43, &
nan, nan, &
nan, nan, &
nan, nan)

end module ciaaw__saw
```

- *ciaaw_saw_capi.f90*: C API for the sat module.

```
module ciaaw__saw_capi
!! Standard Atomic Weights C API - autogenerated.
use iso_c_binding
use ciaaw__saw
implicit none
private

type, public, bind(C) :: ciaaw_saw_capi_element_t
!! Object representing an element.
character(kind=c_char) :: element(25) !! Element name
character(kind=c_char) :: symbol(9) !! Element symbol
integer(c_int) :: z !! Element atomic number
real(c_double) :: saw_min !! Min standard atomic weight
real(c_double) :: saw_max !! Max standard atomic weight
real(c_double) :: saw !! Value standard atomic weight
real(c_double) :: saw_u !! Uncertainty standard atomic weight
real(c_double) :: asaw !! Abridged value standard atomic weight
real(c_double) :: asaw_u !! Abridged uncertainty standard atomic weight
end type

integer(c_int), protected, public, bind(C, name="ciaaw_saw_capi_YEAR") :: ciaaw_saw_
↪capi_YEAR = ciaaw_saw_YEAR

type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_H")␣
↪:: ciaaw_saw_capi_H =&
ciaaw_saw_capi_element_t(&
["h","y","d","r","o","g","e","n",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["H",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_H%z, &
ciaaw_saw_H%saw_max, ciaaw_saw_H%saw_min, ciaaw_saw_H%saw, ciaaw_saw_H%saw_u, ciaaw_
↪saw_H%asaw, ciaaw_saw_H%asaw_u)
```

(continues on next page)

(continued from previous page)

```
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_He")␣
↪:: ciaaw_saw_capi_He =&
ciaaw_saw_capi_element_t(&
["h","e","l","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["H","e",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_He%z, &
ciaaw_saw_He%saw_max, ciaaw_saw_He%saw_min, ciaaw_saw_He%saw, ciaaw_saw_He%saw_u,␣
↪ciaaw_saw_He%asaw, ciaaw_saw_He%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Li")␣
↪:: ciaaw_saw_capi_Li =&
ciaaw_saw_capi_element_t(&
["l","i","t","h","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["L","i",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Li%z, &
ciaaw_saw_Li%saw_max, ciaaw_saw_Li%saw_min, ciaaw_saw_Li%saw, ciaaw_saw_Li%saw_u,␣
↪ciaaw_saw_Li%asaw, ciaaw_saw_Li%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Be")␣
↪:: ciaaw_saw_capi_Be =&
ciaaw_saw_capi_element_t(&
["b","e","r","y","l","l","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["B","e",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Be%z, &
ciaaw_saw_Be%saw_max, ciaaw_saw_Be%saw_min, ciaaw_saw_Be%saw, ciaaw_saw_Be%saw_u,␣
↪ciaaw_saw_Be%asaw, ciaaw_saw_Be%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_B")␣
↪:: ciaaw_saw_capi_B =&
ciaaw_saw_capi_element_t(&
["b","o","r","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["B",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_B%z, &
ciaaw_saw_B%saw_max, ciaaw_saw_B%saw_min, ciaaw_saw_B%saw, ciaaw_saw_B%saw_u, ciaaw_
↪saw_B%asaw, ciaaw_saw_B%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_C")␣
↪:: ciaaw_saw_capi_C =&
ciaaw_saw_capi_element_t(&
["c","a","r","b","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["C",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_C%z, &
ciaaw_saw_C%saw_max, ciaaw_saw_C%saw_min, ciaaw_saw_C%saw, ciaaw_saw_C%saw_u, ciaaw_
↪saw_C%asaw, ciaaw_saw_C%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_N")␣
↪:: ciaaw_saw_capi_N =&
ciaaw_saw_capi_element_t(&
["n","i","t","r","o","g","e","n",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["N",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_N%z, &
ciaaw_saw_N%saw_max, ciaaw_saw_N%saw_min, ciaaw_saw_N%saw, ciaaw_saw_N%saw_u, ciaaw_
↪saw_N%asaw, ciaaw_saw_N%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_O")␣
↪:: ciaaw_saw_capi_O =&
```

(continues on next page)

(continued from previous page)

```
ciaaw_saw_capi_element_t(&
["o","x","y","g","e","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["O",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_O%z, &
ciaaw_saw_O%saw_max, ciaaw_saw_O%saw_min, ciaaw_saw_O%saw, ciaaw_saw_O%saw_u, ciaaw_
↪saw_O%asaw, ciaaw_saw_O%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_F")␣
↪:: ciaaw_saw_capi_F =&
ciaaw_saw_capi_element_t(&
["f","l","u","o","r","i","n","e",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["F",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_F%z, &
ciaaw_saw_F%saw_max, ciaaw_saw_F%saw_min, ciaaw_saw_F%saw, ciaaw_saw_F%saw_u, ciaaw_
↪saw_F%asaw, ciaaw_saw_F%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ne")␣
↪:: ciaaw_saw_capi_Ne =&
ciaaw_saw_capi_element_t(&
["n","e","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["N","e",c_null_char, " "," "," "," "," "], &
ciaaw_saw_Ne%z, &
ciaaw_saw_Ne%saw_max, ciaaw_saw_Ne%saw_min, ciaaw_saw_Ne%saw, ciaaw_saw_Ne%saw_u,␣
↪ciaaw_saw_Ne%asaw, ciaaw_saw_Ne%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Na")␣
↪:: ciaaw_saw_capi_Na =&
ciaaw_saw_capi_element_t(&
["s","o","d","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["N","a",c_null_char, " "," "," "," "," "], &
ciaaw_saw_Na%z, &
ciaaw_saw_Na%saw_max, ciaaw_saw_Na%saw_min, ciaaw_saw_Na%saw, ciaaw_saw_Na%saw_u,␣
↪ciaaw_saw_Na%asaw, ciaaw_saw_Na%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Mg")␣
↪:: ciaaw_saw_capi_Mg =&
ciaaw_saw_capi_element_t(&
["m","a","g","n","e","s","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["M","g",c_null_char, " "," "," "," "," "], &
ciaaw_saw_Mg%z, &
ciaaw_saw_Mg%saw_max, ciaaw_saw_Mg%saw_min, ciaaw_saw_Mg%saw, ciaaw_saw_Mg%saw_u,␣
↪ciaaw_saw_Mg%asaw, ciaaw_saw_Mg%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Al")␣
↪:: ciaaw_saw_capi_Al =&
ciaaw_saw_capi_element_t(&
["a","l","u","m","i","n","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["A","l",c_null_char, " "," "," "," "," "], &
ciaaw_saw_Al%z, &
ciaaw_saw_Al%saw_max, ciaaw_saw_Al%saw_min, ciaaw_saw_Al%saw, ciaaw_saw_Al%saw_u,␣
↪ciaaw_saw_Al%asaw, ciaaw_saw_Al%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Si")␣
↪:: ciaaw_saw_capi_Si =&
ciaaw_saw_capi_element_t(&
["s","i","l","i","c","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
```

(continues on next page)

(continued from previous page)

```
↪" "," "," "," "," "," "], &
["S","i",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Si%z, &
ciaaw_saw_Si%saw_max, ciaaw_saw_Si%saw_min, ciaaw_saw_Si%saw, ciaaw_saw_Si%saw_u,␣
↪ciaaw_saw_Si%asaw, ciaaw_saw_Si%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_P")␣
↪:: ciaaw_saw_capi_P =&
ciaaw_saw_capi_element_t(&
["p","h","o","s","p","h","o","r","o","u","s",c_null_char, " "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["P",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_P%z, &
ciaaw_saw_P%saw_max, ciaaw_saw_P%saw_min, ciaaw_saw_P%saw, ciaaw_saw_P%saw_u, ciaaw_
↪saw_P%asaw, ciaaw_saw_P%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_S")␣
↪:: ciaaw_saw_capi_S =&
ciaaw_saw_capi_element_t(&
["s","u","l","f","u","r",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["S",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_S%z, &
ciaaw_saw_S%saw_max, ciaaw_saw_S%saw_min, ciaaw_saw_S%saw, ciaaw_saw_S%saw_u, ciaaw_
↪saw_S%asaw, ciaaw_saw_S%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Cl")␣
↪:: ciaaw_saw_capi_Cl =&
ciaaw_saw_capi_element_t(&
["c","h","l","o","r","i","n","e",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["C","l",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Cl%z, &
ciaaw_saw_Cl%saw_max, ciaaw_saw_Cl%saw_min, ciaaw_saw_Cl%saw, ciaaw_saw_Cl%saw_u,␣
↪ciaaw_saw_Cl%asaw, ciaaw_saw_Cl%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ar")␣
↪:: ciaaw_saw_capi_Ar =&
ciaaw_saw_capi_element_t(&
["a","r","g","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["A","r",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Ar%z, &
ciaaw_saw_Ar%saw_max, ciaaw_saw_Ar%saw_min, ciaaw_saw_Ar%saw, ciaaw_saw_Ar%saw_u,␣
↪ciaaw_saw_Ar%asaw, ciaaw_saw_Ar%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_K")␣
↪:: ciaaw_saw_capi_K =&
ciaaw_saw_capi_element_t(&
["p","o","t","a","s","s","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["K",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_K%z, &
ciaaw_saw_K%saw_max, ciaaw_saw_K%saw_min, ciaaw_saw_K%saw, ciaaw_saw_K%saw_u, ciaaw_
↪saw_K%asaw, ciaaw_saw_K%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ca")␣
↪:: ciaaw_saw_capi_Ca =&
ciaaw_saw_capi_element_t(&
["c","a","l","c","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["C","a",c_null_char, " "," "," "," "," "," "], &
```

(continues on next page)

(continued from previous page)

```
ciaaw_saw_Ca%z, &
ciaaw_saw_Ca%saw_max, ciaaw_saw_Ca%saw_min, ciaaw_saw_Ca%saw, ciaaw_saw_Ca%saw_u,␣
↪ciaaw_saw_Ca%asaw, ciaaw_saw_Ca%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Sc")␣
↪:: ciaaw_saw_capi_Sc =&
ciaaw_saw_capi_element_t(&
["s","c","a","n","d","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["S","c",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Sc%z, &
ciaaw_saw_Sc%saw_max, ciaaw_saw_Sc%saw_min, ciaaw_saw_Sc%saw, ciaaw_saw_Sc%saw_u,␣
↪ciaaw_saw_Sc%asaw, ciaaw_saw_Sc%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ti")␣
↪:: ciaaw_saw_capi_Ti =&
ciaaw_saw_capi_element_t(&
["t","i","t","a","n","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["T","i",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Ti%z, &
ciaaw_saw_Ti%saw_max, ciaaw_saw_Ti%saw_min, ciaaw_saw_Ti%saw, ciaaw_saw_Ti%saw_u,␣
↪ciaaw_saw_Ti%asaw, ciaaw_saw_Ti%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_V")␣
↪:: ciaaw_saw_capi_V =&
ciaaw_saw_capi_element_t(&
["v","a","n","a","d","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["V",c_null_char, " "," "," "," "," "," "," "], &
ciaaw_saw_V%z, &
ciaaw_saw_V%saw_max, ciaaw_saw_V%saw_min, ciaaw_saw_V%saw, ciaaw_saw_V%saw_u, ciaaw_
↪saw_V%asaw, ciaaw_saw_V%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Cr")␣
↪:: ciaaw_saw_capi_Cr =&
ciaaw_saw_capi_element_t(&
["c","h","r","o","m","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["C","r",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Cr%z, &
ciaaw_saw_Cr%saw_max, ciaaw_saw_Cr%saw_min, ciaaw_saw_Cr%saw, ciaaw_saw_Cr%saw_u,␣
↪ciaaw_saw_Cr%asaw, ciaaw_saw_Cr%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Mn")␣
↪:: ciaaw_saw_capi_Mn =&
ciaaw_saw_capi_element_t(&
["m","a","n","g","a","n","e","s","e",c_null_char, " "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["M","n",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Mn%z, &
ciaaw_saw_Mn%saw_max, ciaaw_saw_Mn%saw_min, ciaaw_saw_Mn%saw, ciaaw_saw_Mn%saw_u,␣
↪ciaaw_saw_Mn%asaw, ciaaw_saw_Mn%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Fe")␣
↪:: ciaaw_saw_capi_Fe =&
ciaaw_saw_capi_element_t(&
["i","r","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["F","e",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Fe%z, &
ciaaw_saw_Fe%saw_max, ciaaw_saw_Fe%saw_min, ciaaw_saw_Fe%saw, ciaaw_saw_Fe%saw_u,␣
```

(continues on next page)

(continued from previous page)

```
↪ciaaw_saw_Fe%asaw, ciaaw_saw_Fe%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Co")␣
↪:: ciaaw_saw_capi_Co =&
ciaaw_saw_capi_element_t(&
["c","o","b","a","l","t",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["C","o",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Co%z, &
ciaaw_saw_Co%saw_max, ciaaw_saw_Co%saw_min, ciaaw_saw_Co%saw, ciaaw_saw_Co%saw_u,␣
↪ciaaw_saw_Co%asaw, ciaaw_saw_Co%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ni")␣
↪:: ciaaw_saw_capi_Ni =&
ciaaw_saw_capi_element_t(&
["n","i","c","k","e","l",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["N","i",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Ni%z, &
ciaaw_saw_Ni%saw_max, ciaaw_saw_Ni%saw_min, ciaaw_saw_Ni%saw, ciaaw_saw_Ni%saw_u,␣
↪ciaaw_saw_Ni%asaw, ciaaw_saw_Ni%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Cu")␣
↪:: ciaaw_saw_capi_Cu =&
ciaaw_saw_capi_element_t(&
["c","o","p","p","e","r",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["C","u",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Cu%z, &
ciaaw_saw_Cu%saw_max, ciaaw_saw_Cu%saw_min, ciaaw_saw_Cu%saw, ciaaw_saw_Cu%saw_u,␣
↪ciaaw_saw_Cu%asaw, ciaaw_saw_Cu%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Zn")␣
↪:: ciaaw_saw_capi_Zn =&
ciaaw_saw_capi_element_t(&
["z","i","n","c",c_null_char, " "," "," "," "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["Z","n",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Zn%z, &
ciaaw_saw_Zn%saw_max, ciaaw_saw_Zn%saw_min, ciaaw_saw_Zn%saw, ciaaw_saw_Zn%saw_u,␣
↪ciaaw_saw_Zn%asaw, ciaaw_saw_Zn%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ga")␣
↪:: ciaaw_saw_capi_Ga =&
ciaaw_saw_capi_element_t(&
["g","a","l","l","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["G","a",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Ga%z, &
ciaaw_saw_Ga%saw_max, ciaaw_saw_Ga%saw_min, ciaaw_saw_Ga%saw, ciaaw_saw_Ga%saw_u,␣
↪ciaaw_saw_Ga%asaw, ciaaw_saw_Ga%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Ge")␣
↪:: ciaaw_saw_capi_Ge =&
ciaaw_saw_capi_element_t(&
["g","e","r","m","a","n","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["G","e",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Ge%z, &
ciaaw_saw_Ge%saw_max, ciaaw_saw_Ge%saw_min, ciaaw_saw_Ge%saw, ciaaw_saw_Ge%saw_u,␣
↪ciaaw_saw_Ge%asaw, ciaaw_saw_Ge%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_As")␣
```

(continues on next page)

(continued from previous page)

```
↪:: ciaaw_saw_capi_As =&
ciaaw_saw_capi_element_t(&
["a","r","s","e","n","i","c",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["A","s",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_As%z, &
ciaaw_saw_As%saw_max, ciaaw_saw_As%saw_min, ciaaw_saw_As%saw, ciaaw_saw_As%saw_u,␣
↪ciaaw_saw_As%asaw, ciaaw_saw_As%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Se")␣
↪:: ciaaw_saw_capi_Se =&
ciaaw_saw_capi_element_t(&
["s","e","l","e","n","i","u","m",c_null_char, " "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["S","e",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Se%z, &
ciaaw_saw_Se%saw_max, ciaaw_saw_Se%saw_min, ciaaw_saw_Se%saw, ciaaw_saw_Se%saw_u,␣
↪ciaaw_saw_Se%asaw, ciaaw_saw_Se%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Br")␣
↪:: ciaaw_saw_capi_Br =&
ciaaw_saw_capi_element_t(&
["b","r","o","m","i","n","e",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["B","r",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Br%z, &
ciaaw_saw_Br%saw_max, ciaaw_saw_Br%saw_min, ciaaw_saw_Br%saw, ciaaw_saw_Br%saw_u,␣
↪ciaaw_saw_Br%asaw, ciaaw_saw_Br%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Kr")␣
↪:: ciaaw_saw_capi_Kr =&
ciaaw_saw_capi_element_t(&
["k","r","y","p","t","o","n",c_null_char, " "," "," "," "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["K","r",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Kr%z, &
ciaaw_saw_Kr%saw_max, ciaaw_saw_Kr%saw_min, ciaaw_saw_Kr%saw, ciaaw_saw_Kr%saw_u,␣
↪ciaaw_saw_Kr%asaw, ciaaw_saw_Kr%asaw_u)
type(ciaaw_saw_capi_element_t), protected, public, bind(C, name="ciaaw_saw_capi_Tc")␣
↪:: ciaaw_saw_capi_Tc =&
ciaaw_saw_capi_element_t(&
["t","e","c","h","n","e","t","i","u","m",c_null_char, " "," "," "," "," "," "," "," ",
↪" "," "," "," "," "," "], &
["T","c",c_null_char, " "," "," "," "," "," "], &
ciaaw_saw_Tc%z, &
ciaaw_saw_Tc%saw_max, ciaaw_saw_Tc%saw_min, ciaaw_saw_Tc%saw, ciaaw_saw_Tc%saw_u,␣
↪ciaaw_saw_Tc%asaw, ciaaw_saw_Tc%asaw_u)

end module ciaaw__saw_capi
```

4.1.2 C

- *ciaaw.h*: Main C header for the whole library.

```
/**
 * @file
 * @brief Main C header for the CIAAW library.
 */
#ifndef CIAAW_H
#define CIAAW_H

#include "ciaaw_version.h"
#include "ciaaw_saw.h"

#endif
```

SAW (Standard Atomic Weights)

- *ciaaw_saw.h*: C header.

```
/**
* @file
* @brief Standard Atomic Weights - autogenerated.
*/

#ifndef CIAAW_SAW_H
#define CIAAW_SAW_H
#if _MSC_VER
#define ADD_IMPORT __declspec(dllimport)
#else
#define ADD_IMPORT
#endif
struct ciaaw_saw_capi_element_t{
    char element[25];
    char symbol[9];
    int z;
    double saw_min;
    double saw_max;
    double saw;
    double saw_u;
    double asaw;
    double asaw_u;
};
ADD_IMPORT extern const int ciaaw_saw_capi_YEAR;

ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_H;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_He;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Li;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Be;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_B;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_C;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_N;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_O;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_F;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ne;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Na;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Mg;
```

(continues on next page)

(continued from previous page)

```
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Al;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Si;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_P;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_S;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Cl;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ar;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_K;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ca;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Sc;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ti;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_V;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Cr;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Mn;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Fe;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Co;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ni;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Cu;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Zn;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ga;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Ge;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_As;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Se;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Br;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Kr;
ADD_IMPORT extern const struct ciaaw_saw_capi_element_t ciaaw_saw_capi_Tc;

#endif
```

4.2 pyciaaw

4.2.1 SAW (Standard atomic weights)

All constant as declared in the *ciaaw* are inserted at the top level of the module. C extension for saw.

BIBLIOGRAPHY

[1] Thomas Prohaska, Johanna Irrgeher, Jacqueline Benefield, John K. Böhlke, Lesley A. Chesson, Tyler B. Coplen, Tiping Ding, Philip J. H. Dunn, Manfred Gröning, Norman E. Holden, Harro A. J. Meijer, Heiko Moossen, Antonio Possolo, Yoshio Takahashi, Jochen Vogl, Thomas Walczyk, Jun Wang, Michael E. Wieser, Shigekazu Yoneda, Xiang-Kun Zhu, and Juris Meija. Standard atomic weights of the elements 2021 (iupac technical report). *Pure and Applied Chemistry*, 94(5):573–600, 2022. URL: https://doi.org/10.1515/pac-2019-0603, doi:doi:10.1515/pac-2019-0603.

[2] Adriaan M. H. van der Veen, Juris Meija, Antonio Possolo, and David Brynn Hibbert. Interpretation and use of standard atomic weights (iupac technical report). *Pure and Applied Chemistry*, 93(5):629–646, 2021. URL: https://doi.org/10.1515/pac-2017-1002, doi:doi:10.1515/pac-2017-1002.

PYTHON MODULE INDEX

INDEX