NAME

ciaaw - library for isotopic abundances and standard atomic weights

LIBRARY

ciaaw (**-libciaaw**, **-lciaaw**)

SYNOPSIS

```
use ciaaw
include "ciaaw.h"
import pyciaaw
```

DESCRIPTION

ciaaw is a Fortran library providing the standard and abridged atomic weights, the isotopic abundance and the isotopes' standard atomic weights. The data are taken from http://ciaaw.org. C API allows usage from C, or can be used as a basis for other wrappers. Python wrapper allows easy usage from Python.

What have been implemented:

   o SAW   Standard Atomic Weights.

   o ICE   Isotopic Composition of the Element

   o NAW   Nuclides Atomic Weight.

The latest standard atomic weights were released in 2021 by the *ciaaw* (https://www.ciaaw.org). All the values for the atomic weights are provided as double precision reals. The standard atomic weights (or realtive atomic mass), A_r(E), are extracted from table 1 from Prohaska et al. (IUPAC Technical Report **94**(5):573–600). For the elements that feature an interval for the standard atomic weight, the mean value and the uncertainty are computed using formulas defined in [2]. The standard atomic weights are a dimensionless quantity and thus they need to be multiplied by the molar mass constant Mu in order to get the value in g.mol-1. See codata for physical constants.

The latest isotopic compositions were released in 2013 by the *ciaaw* (https://www.ciaaw.org). All the values for the compositions are provided as double precision reals. The isotopic compositions of the element, are extracted from table 1 from Meija et al. (IUPAC Technical Report. **88**(3):293–306).

The latest atomic weights for nuclides were released in 2020 by *ciaaw* https://www.ciaaw.org from Huang et al. (AME 2020 **45**(3):030002). All the values for the nuclide atomic weights are provided as double precision reals.

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.

   • (ciaaw_)get_saw

   • (ciaaw_)get_ice

   • (ciaaw_)get_nice

   • (ciaaw_)get_naw

   • (ciaaw_)get_nnaw

NOTES

To **use** *ciaaw* within your fpm project, add the following to your fpm.toml file:

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

EXAMPLES

Example in Fortran:

```
program example_in_f
```

```fortran
            use ciaaw
            implicit none

            character(len=8) :: s

            ! ASAW = Abridged Standard Atomic Weight
            ! SAW  = Standard Atomic Weight
            ! ICE  = Isotopic Composition of the Element
            ! NAW  = Nuclide Atomic Weight
            ! U    = Uncertainty

            print '(A)', '########## CIAAW VERSION ##########'
            print *, "version ", get_version()

            print '(A)', '########## CIAAW SAW ##########'
            print '(A10, F10.5)', 'ASAW H   = ', get_saw("H", abridged=.true.)
            print '(A10, F10.5)', 'U ASAW H = ', get_saw("H", uncertainty=.true.)
            print '(A10, F10.5)', 'SAW H    = ', get_saw("H", abridged = .false.)
            print '(A10, F10.5)', 'U SAW H  = ', get_saw("H", abridged = .false., un
            print '(A10, F10.5)', 'ASAW T   = ', get_saw("Tc", abridged=.true.)

            print '(A)', '########## CIAAW ICE ##########'
            print '(A, I3)',      'N ICE H   = ', get_nice("H")
            print '(A, F12.6)',   'ICE H 1   = ', get_ice("H", A=1)
            print '(A, ES23.16)', 'U ICE H 1 = ', get_ice("H", A=1, uncertainty=.tru
            print '(A, F12.6)',   'ICE H 2   = ', get_ice("H", A=2)
            print '(A, ES23.16)', 'U ICE H 2 = ', get_ice("H", A=2, uncertainty=.tru
            print '(A, I3)',      'N ICE Tc  = ', get_nice("Tc")
            print '(A, I3)',      'N ICE C   = ', get_nice("C")

            print '(A)', '########## CIAAW NAW ##########'
            print '(A, ES23.16)',  'NAW H 2    = ', get_naw("H", A=2)
            print '(A, ES23.16)',  'U NAW H 2  = ', get_naw("H", A=2, uncertainty=.
            print '(A, I3)',       'N NAW Tc   = ', get_nnaw("Tc")
            end program
```

Example in C:

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


            // ASAW = Abridged Standard Atomic Weight
            // SAW  = Standard Atomic Weight
            // ICE  = Isotopic Composition of the Element
            // NAW  = Nuclide Atomic Weight
            // U    = Uncertainty

            int main(void){
                printf("%s0, "########## CIAAW VERSION ##########");
                printf("version %s0, ciaaw_get_version());
```

```
                    printf("%s0, "########## CIAAW SAW ##########");
                    printf("%s %10.5f0, "ASAW H  = ", ciaaw_get_saw("H", 1, true, false)
                    printf("%s %10.5f0, "U ASAW H = ", ciaaw_get_saw("H", 1, true, true))
                    printf("%s %10.5f0, "SAW H   = ", ciaaw_get_saw("H", 1, false, false
                    printf("%s %10.5f0, "U SAW H  = ", ciaaw_get_saw("H", 1, false, true)
                    printf("%s %10.5f0, "ASAW Tc  = ", ciaaw_get_saw("Tc", 2, true, false

                    printf("%s0, "########## CIAAW ICE ##########");
                    printf("%s %d0,      "N ICE H     = ", ciaaw_get_nice("H", 1));
                    printf("%s %12.6f0, "ICE H 1     = ", ciaaw_get_ice("H", 1, 1, false
                    printf("%s %23.16e0,"U ICE H 1   = ", ciaaw_get_ice("H", 1, 1, true)
                    printf("%s %12.6f0, "ICE H 2     = ", ciaaw_get_ice("H", 1, 2, false
                    printf("%s %23.16e0,"U ICE H 2   = ", ciaaw_get_ice("H", 1, 2, true)
                    printf("%s %d0,      "N ICE Tc    = ", ciaaw_get_nice("Tc", 2));
                    printf("%s %d0,      "N ICE C     = ", ciaaw_get_nice("C", 1));

                    printf("%s0, "########## CIAAW NAW ##########");
                    printf("%s %23.16f0, "NAW H 2      = ", ciaaw_get_naw("H", 1, 2, false
                    printf("%s %23.16e0, "U NAW H 2    = ", ciaaw_get_naw("H", 1, 2, true
                    printf("%s %d0,        "N NAW Tc    = ", ciaaw_get_nnaw("Tc", 2));
                    return EXIT_SUCCESS;
                    }
```

Example in Python:

```python
        import pyciaaw

        # ASAW = Abridged Standard Atomic Weight
        # SAW  = Standard Atomic Weight
        # ICE  = Isotopic Composition of the Element
        # NAW  = Nuclide Atomic Weight
        # U    = Uncertainty

        print("########## CIAAW VERSION ##########")
        print("version ", pyciaaw.__version__)

        print("########## CIAAW SAW  ##########")
        print("ASAW H  = ", pyciaaw.get_saw("H"))
        print("U ASAW H = ", pyciaaw.get_saw("H", uncertainty=True))
        print("SAW H   = ", pyciaaw.get_saw("H", abridged=False, uncertainty=Fal
        print("U SAW H  = ", pyciaaw.get_saw("H", abridged=False, uncertainty=Tru
        print("ASAW Tc  = ", pyciaaw.get_saw("Tc"))


        print("########## CIAAW ICE  ##########")
        print("N ICE H  = ", pyciaaw.get_nice("H"))
        print('ICE H 1   = ', pyciaaw.get_ice("H", A=1))
        print('U ICE H 1 = ', pyciaaw.get_ice("H", A=1, uncertainty=True))
        print('ICE H 2   = ', pyciaaw.get_ice("H", A=2))
        print('U ICE H 2 = ', pyciaaw.get_ice("H", A=2, uncertainty=True))
        print("N ICE Tc  = ", pyciaaw.get_nice("Tc"))
        print("N ICE C   = ", pyciaaw.get_nice("C"))

        print("########## CIAAW NAW  ##########")
        print('NAW H 2   = ', pyciaaw.get_naw("H", A=2))
```

```
print('U NAW H 2 = ', pyciaaw.get_naw("H", A=2, uncertainty=True))
print("N NAW Tc  = ", pyciaaw.get_nnaw("Tc"))
```

SEE ALSO

> **gsl**(3), **codata**(3), **ciaaw_get_version**(3), **ciaaw_get_saw**(3) **ciaaw_get_ice**(3), **ciaaw_get_nice**(3),
> **ciaaw_get_naw**(3), **ciaaw_get_naw**(3)