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:

- **SAW** Standard Atomic Weights.
- **ICE** Isotopic Composition of the Element
- **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.

Fortran API

- **function get_version()result(fptr)**
  Get the version
  - **character(len=:), pointer :: fptr**
    Fortran pointer to a string indicating the version..
- **function is_in_pt(z)result(res)**
  Check if the atomic number z is in the periodic table
  - **integer(int32), intent(in) :: z**
    Atomic number
  - **logical :: res**
    True or False
- **function get_z_by_symbol(s)result(res)**
  Get the atomic number z of the element defined by the symbol s.
  - **character(len=*), intent(in) :: s**
    Element symbol

- **integer(int32) :: res**
  >0 if found and **-1** if not found.

o subroutine print_periodic_table()
Print periodic table.

o function get_saw(s, abridged, uncertainty)result(res)
Get the standard atomic weight for the element s.

- **character(len=*), intent(in) :: s**
  Element symbol.
- **logical, intent(in), optional :: abridged**
  Set to False if the abridged value is not desired. Default to TRUE.
- **logical, intent(in), optional :: uncertainty**
  Set to True if the uncertainty is desired. Default to FALSE.
- **real(dp) :: res**
  NaN if the provided element is incorrect or **-1** if the element does not have a SAW.

o function get_ice(s, A, uncertainty)result(res)
Get the isotopic composition of the element s for the mass number A.

- **character(len=*), intent(in) :: s**
  Element symbol.
- **integer(int32), intent(in) :: A**
  Mass number.
- **logical, intent(in), optional :: uncertainty**
  Set to True if the uncertainty is desired. Default to FALSE.
- **real(dp) :: res**
  NaN if the provided element or the mass number A are incorrect or **-1** if the element does not have an ICE.

o function get_nice(s)result(res)
Get the number of isotopes in ICE of the element s.

- **character(len=*), intent(in) :: s**
  Element symbol.
- **integer(int32) :: res**
  >0 if found or **-1** if not found.

o function get_naw(s, A, uncertainty)result(res)
Get the atomic weight of the nuclide s for the mass number A.

- **character(len=*), intent(in) :: s**
  Element symbol.
- **integer(int32), intent(in) :: A**
  Mass number.
- **logical, intent(in), optional :: uncertainty**
  Flag for returning the uncertainty instead of the value. Default to FALSE.
- **real(dp) :: res**
  NaN if the provided element or A are incorrect or **-1** if the element does not have an NAW.

o function get_nnaw(s)result(res)
Get the number of nuclides in NAW of the element s.

o character(len=*), intent(in) :: s
Element symbol.

o integer(int32) :: res
>O if found or **-1** if not found.

C API

- char* **ciaaw_get_version**(void)
- double **ciaaw_get_saw**(char *s, int n, bool abridged, bool uncertainty)
- double **ciaaw_get_ice**(char *s, int n, int A, bool uncertainty)
- int **ciaaw_get_nice**(char *s, int n)
- double **ciaaw_get_naw**(char *s, int n, int A, bool uncertaintuy)
- int **ciaaw_get_nnaw**(char *s, int n)

Python wrappers

- **get_saw**(s: str, abridged: bool=True, uncertainty: bool=False)->float
- **get_ice**(s:str, A:int, uncertainty: bool=False)->float
- **get_nice**(s:str)->int
- **get_naw**(s:str, A:int, uncertainty: bool=False)->float
- **get_nnaw**(s:str)->int

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" }
```

dp stands for double precision and it is an alias to real64 from the iso_fortran_env module.

The definitions of the acronyms:

o ASAW
Abridged Standard Atomic Weight

o SAW Standard Atomic Weight

o ICE Isotopic Composition of the Element

o NAW Nuclide Atomic Weight

o U Uncertainty

The definitions of the common variables:

o s Element

o Z Atomic number

o A Mass number

o u Uncertainty

o ab Abridged

o res Return values

EXAMPLES

Example in Fortran:

```
program example_in_f
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=.tr
print '(A, I3)',      'N NAW Tc    = ', get_nnaw("Tc")

end program
```

Example in 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:

```
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=Fals
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)