

Package ‘isocalcR’

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Type Package

Title Isotope Calculations in R

Version 0.1.1

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Description Perform common calculations based on published stable isotope theory, such as calculating carbon isotope discrimination and intrinsic water use efficiency from wood or leaf carbon isotope composition. See Mathias and Hudiburg (2022) in Global Change Biology <[doi:10.1111/gcb.16407](https://doi.org/10.1111/gcb.16407)>.

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URL <https://github.com/justinmathias/isocalcR>

BugReports <https://github.com/justinmathias/isocalcR/issues>

Depends R (>= 4.0.0)

Encoding UTF-8

Language en-US

LazyData true

Suggests rmarkdown, knitr, testthat (>= 3.0.0), ggplot2, tidyr, dplyr

VignetteBuilder knitr

Config/testthat/edition 3

RoxygenNote 7.2.1

NeedsCompilation no

Repository CRAN

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CO2data	<i>CO2data</i>
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Description

Compiled records of atmospheric CO2 concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. Data are from Belmecheri, Lavergne, 2020, Dendrochronologia. Updated based on their methodology beyond C.E. 2019.

Usage

data(CO2data)

Format

A data frame with 2023 rows and 3 variables:
yr Year of CO2 and d13CO2 measurement
Ca Atmospheric CO2 concentration, in ppm
d13C.atm Atmospheric d13CO2, in per mille, ‰

Source

<https://www.sciencedirect.com/science/article/abs/pii/S1125786520300874>

References

Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO2 concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. Dendrochronologia, 63, 125748.

Examples

data(CO2data)
head(CO2data)
tail(CO2data)

custom.calc

custom.calc

Description

Calculates D13C, Ci, CiCa, diffCaCi, or iWUE with user specified values of d13C.plant, d13CO2.atm, atmospheric CO2, temperature, and elevation. The user can also specify whether to calculate each physiological index using the 'simple', 'photorespiration', or 'mesophyll' formulation in all calculations where Ci is computed. Method defaults to 'simple' assuming 'leaf' tissue and incorporates an apparent fractionation by Rubisco, b, of 27 permille (Cernusak and Ubierna 2022). If 'wood' tissue is supplied as an argument in the 'simple' method, the apparent fractionation by Rubisco, b, is updated to 25.5 permille (Cernusak and Ubierna 2022).

Usage

```
custom.calc(
  d13C.plant,
  d13C.atm,
  frac = 0,
  outvar = "D13C",
  Ca = NULL,
  elevation = NULL,
  temp = NULL,
  method = "simple",
  tissue = "leaf"
)
```

Arguments

d13C.plant	Measured plant tissue carbon isotope signature, per mille (‰)
d13C.atm	Atmospheric d13CO2, per mille (‰)
frac	Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)
outvar	Variable of interest to calculate from the following: D13C, Ci, CiCa, diffCaCi, or iWUE. Defaults to D13C.
Ca	Atmospheric CO2 concentration (ppm).
elevation	Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
temp	Leaf temperature (°C)
method	Method to calculate iWUE (simple, photorespiration, or mesophyll). Defaults to 'simple'. See Laverne et al. 2022, Ma et al. 2021, Gong et al. 2022.
tissue	Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to 'leaf'.

Value

One of the specified outvars: D13C (permille), Ci (ppm), CiCa (unitless), diffCaCi (ppm), or iWUE (micromol CO₂ per mol H₂O). Defaults to 'D13C'.

References

- Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Commun. Mass Spectrom.*, 19, 1381–1391.
- Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO₂ concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. *Dendrochronologia*, 63, 125748.
- Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. & Long, S.P. (2001). Improved temperature response functions for models of Rubisco-limited photosynthesis. *Plant, Cell Environ.*, 24, 253–259.
- Craig, H. (1953). The geochemistry of the stable carbon isotopes. *Geochim. Cosmochim. Acta*, 3, 53–92.
- Cernusak, L. A. & Ubierna, N. Carbon Isotope Effects in Relation to CO₂ Assimilation by Tree Canopies. in *Stable Isotopes in Tree Rings: inferring physiological, climatic, and environmental responses* 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.
- Davies, J.A. & Allen, C.D. (1973). Equilibrium, Potential and Actual Evaporation from Cropped Surfaces in Southern Ontario. *J. Appl. Meteorol.*, 12, 649–657.
- Farquhar, G., O’Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. *Aust. J. Plant Physiol.*, 9, 121–137.
- Frank, D.C., Poulter, B., Saurer, M., Esper, J., Huntingford, C., Helle, G., et al. (2015). Water-use efficiency and transpiration across European forests during the Anthropocene. *Nat. Clim. Chang.*, 5, 579–583.
- Gong, X. Y. et al. Overestimated gains in water-use efficiency by global forests. *Glob. Chang. Biol.* 1–12 (2022) doi:10.1111/gcb.16221.
- Lavergne, A. et al. Global decadal variability of plant carbon isotope discrimination and its link to gross primary production. *Glob. Chang. Biol.* 28, 524–541 (2022).
- Ma, W. T. et al. Accounting for mesophyll conductance substantially improves ¹³C-based estimates of intrinsic water-use efficiency. *New Phytol.* 229, 1326–1338 (2021).
- Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. *Energy Convers. Manag.*, 49, 1098–1110.
- Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C₃ plants. *Plant. Cell Environ.*, 37, 1494–1498.

Examples

```
custom.calc(d13C.plant = -27, d13C.atm = -8.7)
```

<i>d13C.to.Ci</i>	<i>d13C.to.Ci</i>
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Description

Calculates leaf intercellular CO₂ concentration given plant tissue d13C signature. Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf Ci. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

Usage

```
d13C.to.Ci(
  d13C.plant,
  year,
  elevation,
  temp,
  method = "simple",
  tissue = "leaf",
  frac = 0
)
```

Arguments

<i>d13C.plant</i>	Measured plant tissue carbon isotope signature, per mille (‰)
<i>year</i>	Year to which the sample corresponds
<i>elevation</i>	Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
<i>temp</i>	Leaf temperature (°C)
<i>method</i>	Method to calculate CiCa (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
<i>tissue</i>	Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to "leaf".
<i>frac</i>	Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)

Value

The concentration of leaf internal CO₂ (ppm)

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Commun. Mass Spectrom.*, 19, 1381–1391.

- Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO₂ concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. *Dendrochronologia*, 63, 125748.
- Bernacchi, C.J., Singaas, E.L., Pimentel, C., Portis Jr, A.R. & Long, S.P. (2001). Improved temperature response functions for models of Rubisco-limited photosynthesis. *Plant, Cell Environ.*, 24, 253–259.
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- Farquhar, G., O’Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. *Aust. J. Plant Physiol.*, 9, 121–137.
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- Gong, X. Y. et al. Overestimated gains in water-use efficiency by global forests. *Glob. Chang. Biol.* 1–12 (2022) doi:10.1111/gcb.16221.
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- Ma, W. T. et al. Accounting for mesophyll conductance substantially improves ¹³C-based estimates of intrinsic water-use efficiency. *New Phytol.* 229, 1326–1338 (2021).
- Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. *Energy Convers. Manag.*, 49, 1098–1110.
- Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C₃ plants. *Plant. Cell Environ.*, 37, 1494–1498.

Examples

```
d13C.to.Ci(d13C.plant = -27,
           year = 2015,
           elevation = 900,
           temp = 24,
           method = "simple",
           tissue = "leaf")
```

```
d13C.to.Ci(d13C.plant = -27,
           year = 2015,
           elevation = 900,
           temp = 24,
           method = "simple",
           tissue = "wood")
```

```
d13C.to.Ci(d13C.plant = -27,
           year = 2015,
           elevation = 900,
           temp = 24,
           method = "photorespiration")
```

d13C.to.CiCa

d13C.to.CiCa

Description

Calculates the ratio of the concentration of leaf intercellular to atmospheric CO₂, unitless. Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf C_i, and subsequently C_iCa. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

Usage

```
d13C.to.CiCa(
  d13C.plant,
  year,
  elevation,
  temp,
  method = "simple",
  tissue = "leaf",
  frac = 0
)
```

Arguments

d13C.plant	Measured plant tissue carbon isotope signature, per mille (‰)
year	Year to which the sample corresponds
elevation	Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
temp	Leaf temperature (°C)
method	Method to calculate C _i Ca (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
tissue	Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to "leaf".
frac	Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)

Value

The ratio of leaf intercellular to atmospheric CO₂ (Ci/Ca), unitless

References

- Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Commun. Mass Spectrom.*, 19, 1381–1391.
- Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO₂ concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. *Dendrochronologia*, 63, 125748.
- Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. & Long, S.P. (2001). Improved temperature response functions for models of Rubisco-limited photosynthesis. *Plant, Cell Environ.*, 24, 253–259.
- Craig, H. (1953). The geochemistry of the stable carbon isotopes. *Geochim. Cosmochim. Acta*, 3, 53–92.
- Cernusak, L. A. & Ubierna, N. Carbon Isotope Effects in Relation to CO₂ Assimilation by Tree Canopies. in *Stable Isotopes in Tree Rings: inferring physiological, climatic, and environmental responses* 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.
- Davies, J.A. & Allen, C.D. (1973). Equilibrium, Potential and Actual Evaporation from Cropped Surfaces in Southern Ontario. *J. Appl. Meteorol.*, 12, 649–657.
- Farquhar, G., O’Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. *Aust. J. Plant Physiol.*, 9, 121–137.
- Frank, D.C., Poulter, B., Saurer, M., Esper, J., Huntingford, C., Helle, G., et al. (2015). Water-use efficiency and transpiration across European forests during the Anthropocene. *Nat. Clim. Chang.*, 5, 579–583.
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- Lavergne, A. et al. Global decadal variability of plant carbon isotope discrimination and its link to gross primary production. *Glob. Chang. Biol.* 28, 524–541 (2022).
- Ma, W. T. et al. Accounting for mesophyll conductance substantially improves ¹³C-based estimates of intrinsic water-use efficiency. *New Phytol.* 229, 1326–1338 (2021).
- Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. *Energy Convers. Manag.*, 49, 1098–1110.
- Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C₃ plants. *Plant. Cell Environ.*, 37, 1494–1498.

Examples

```
d13C.to.CiCa(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
```

```
tissue = "leaf")

d13C.to.CiCa(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "wood")

d13C.to.CiCa(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "photorespiration")
```

d13C.to.D13C

*d13C.to.D13C***Description**

Calculates leaf carbon isotope discrimination given plant tissue d13C signature.

Usage

```
d13C.to.D13C(d13C.plant, year, frac = 0)
```

Arguments

d13C.plant	Measured plant tissue carbon isotope signature, per mille (‰)
year	Year to which the sample corresponds
frac	Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material with no post-photosynthetic fractionation. User should supply reasonable value if leaf fractionation present or if samples are from wood (generally -1.9 - -2.1).

Value

Carbon isotope discrimination in units of per mille (‰).

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Commun. Mass Spectrom.*, 19, 1381–1391.

Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO₂ concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. *Dendrochronologia*, 63, 125748.

Craig, H. (1953). The geochemistry of the stable carbon isotopes. *Geochim. Cosmochim. Acta*, 3, 53–92.

Cernusak, L. A. & Ubierna, N. Carbon Isotope Effects in Relation to CO₂ Assimilation by Tree Canopies. in *Stable Isotopes in Tree Rings: inferring physiological, climatic, and environmental responses* 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.

Farquhar, G., O’Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. *Aust. J. Plant Physiol.*, 9, 121–137.

Frank, D.C., Poulter, B., Saurer, M., Esper, J., Huntingford, C., Helle, G., et al. (2015). Water-use efficiency and transpiration across European forests during the Anthropocene. *Nat. Clim. Chang.*, 5, 579–583.

Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C₃ plants. *Plant. Cell Environ.*, 37, 1494–1498.

Examples

```
d13C.to.D13C(d13C.plant = -27, year = 2015)
```

<code>d13C.to.diffCaCi</code>	<i>d13C.to.diffCaCi</i>
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Description

Calculates the difference between the atmospheric CO₂ concentration and the leaf intercellular CO₂ concentration in parts per mil (ppm). Defaults to the ‘simple’ formulation (See Lavergne et al. 2022) and ‘leaf’ tissue to calculate leaf C_i, and subsequently diffCaCi. Under the ‘simple’ formulation the apparent fractionation by Rubisco is 27 permille if from ‘leaf’ tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

Usage

```
d13C.to.diffCaCi(  
  d13C.plant,  
  year,  
  elevation,  
  temp,  
  method = "simple",  
  tissue = "leaf",  
  frac = 0  
)
```

Arguments

d13C.plant	Measured plant tissue carbon isotope signature, per mille (‰)
year	Year to which the sample corresponds
elevation	Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
temp	Leaf temperature (°C)
method	Method to calculate CiCa (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
tissue	Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to "leaf".
frac	Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)

Value

The difference between atmospheric and leaf intercellular CO₂ concentrations (ppm).

References

- Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Commun. Mass Spectrom.*, 19, 1381–1391.
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- Craig, H. (1953). The geochemistry of the stable carbon isotopes. *Geochim. Cosmochim. Acta*, 3, 53–92.
- Cernusak, L. A. & Ubierna, N. Carbon Isotope Effects in Relation to CO₂ Assimilation by Tree Canopies. in *Stable Isotopes in Tree Rings: inferring physiological, climatic, and environmental responses* 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.
- Davies, J.A. & Allen, C.D. (1973). Equilibrium, Potential and Actual Evaporation from Cropped Surfaces in Southern Ontario. *J. Appl. Meteorol.*, 12, 649–657.
- Farquhar, G., O’Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. *Aust. J. Plant Physiol.*, 9, 121–137.
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Lavergne, A. et al. Global decadal variability of plant carbon isotope discrimination and its link to gross primary production. *Glob. Chang. Biol.* 28, 524–541 (2022).

Ma, W. T. et al. Accounting for mesophyll conductance substantially improves ^{13}C -based estimates of intrinsic water-use efficiency. *New Phytol.* 229, 1326–1338 (2021).

Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. *Energy Convers. Manag.*, 49, 1098–1110.

Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C_3 plants. *Plant. Cell Environ.*, 37, 1494–1498.

Examples

```
d13C.to.diffCaCi(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "leaf")
```

```
d13C.to.diffCaCi(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "wood")
```

```
d13C.to.diffCaCi(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "photorespiration")
```

d13C.to.iWUE

d13C.to.iWUE

Description

Calculates leaf intrinsic water use efficiency given plant tissue d^{13}C signature. Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf C_i , and subsequently iWUE. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

Usage

```
d13C.to.iWUE(
  d13C.plant,
  year,
  elevation,
  temp,
  method = "simple",
  tissue = "leaf",
  frac = 0
)
```

Arguments

d13C.plant	Measured plant tissue carbon isotope signature, per mille (‰)
year	Year to which the sample corresponds
elevation	Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
temp	Leaf temperature (°C)
method	Method to calculate iWUE (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
tissue	Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to "leaf".
frac	Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)

Value

Intrinsic water use efficiency in units of micromol CO₂ per mol H₂O.

References

- Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Commun. Mass Spectrom.*, 19, 1381–1391.
- Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO₂ concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. *Dendrochronologia*, 63, 125748.
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- Ma, W. T. et al. Accounting for mesophyll conductance substantially improves ^{13}C -based estimates of intrinsic water-use efficiency. *New Phytol.* 229, 1326–1338 (2021).
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Examples

```
d13C.to.iWUE(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "leaf")
```

```
d13C.to.iWUE(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "wood")
```

```
d13C.to.iWUE(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "photorespiration")
```

piru13C

piru13C

Description

Accompanying tree ring carbon isotope signature data for "Mathias, J.M. & Thomas, R.B. Disentangling the effects of acidic air pollution, atmospheric CO₂, and climate change on recent growth of red spruce trees in the Central Appalachian Mountains. Glob. Chang. Biol. 24, 3938–3953 (2018).".

Usage

```
data(piru13C)
```

Format

A data frame with 223 rows and 6 variables:

Year Year of sample

Site Study location name

wood.d13C Measured tree ring (i.e. wood) d13C, in per mille, ‰

MGT_C Mean growing season temperature, °C

Elevation_m Elevation of study location, meters

frac Leaf-to-wood fractionation factor

Source

<https://onlinelibrary.wiley.com/doi/full/10.1111/gcb.14273>

References

Mathias, J.M. & Thomas, R.B. Disentangling the effects of acidic air pollution, atmospheric CO₂, and climate change on recent growth of red spruce trees in the Central Appalachian Mountains. Glob. Chang. Biol. 24, 3938–3953 (2018).

Examples

```
data(piru13C)
head(piru13C)
```

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