Package 'iapws'

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of Water and Steam
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Description Implementation of some of the formulations for the thermodynamic and transport properties released by the International Association for the Properties of Water and Steam (IAPWS). More specifically, the releases R1-76(2014), R5-85(1994), R6-95(2018), R7-97(2012), R8-97, R9-97, R10-06(2009), R11-07(2019), R12-08, R15-11, R16-17(2018), R17-20 and R18-21 at http://iapws.org .
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Author Jonathan Debove [aut, cre]
Maintainer Jonathan Debove <jondebove@gmail.com></jondebove@gmail.com>
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heavy17 IAPWS-17 Formulation in Single Phase Regions

Description

Compute thermodynamic and transport properties of heavy water and steam using the IAPWS formulation 2017.

Usage

```
heavy17(what, p, t, rho, state = NULL)
```

Arguments

what	a character vector listing the output properties. See Details for available properties.
р	a numeric vector giving the pressure values in MPa.
t	a numeric vector giving the temperature values in K.
rho	a numeric vector giving the density values in kg/m ³ .
state	NULL or a character vector giving the physical state. One of "liquid", "gas" or "supercritical". In case of NULL, the state is determined by the function heavy17_state().

Details

- "f": the specific free energy in kJ/kg.
- "g": the specific Gibbs enthalpy in kJ/kg.
- "u": the specific internal energy in kJ/kg.
- "h": the specific enthalpy in kJ/kg.
- "s": the specific entropy in kJ/K/kg.
- "t": the temperature in K.
- "p": the pressure in MPa.
- "v": the specific volume in m³/kg.
- "rho": the mass density in kg/m³.
- "cv": the specific isochoric heat capacity in kJ/K/kg.
- "cp": the specific isobaric heat capacity in kJ/K/kg.
- "alpha": the expansion coefficient in 1/K
- "beta": the pressure coefficient in MPa/K.
- "kappat": the isothermal compressibility in 1/MPa.

heavy17

- "w": the speed of sound in m/s.
- "eta": the dynamic viscosity in μ Pa.s.
- "lambda": the thermal conductivity in mW/K/m.

A valid pair of p, rho and t is needed: either (p, t) or (rho, t).

Value

A numeric matrix of dimension c(n, length(what)) with n the maximum length of either rho, p, t or state.

Note

Computing several properties in a single call may be more efficient than separately because most of the computation time is shared.

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R16-17(2018), Revised Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water.

International Association for the Properties of Water and Steam, IAPWS R17-20, Release on the IAPWS Formulation 2020 for the Viscosity of Heavy Water.

International Association for the Properties of Water and Steam, IAPWS R18-21, Release on the IAPWS Formulation 2021 for the Thermal Conductivity of Heavy Water.

```
# IAPWS-17 Tab. 7
M <- 20.027508 # g/mol
tab <- heavy17(c("p", "cv", "w", "s"),
               t = c(300, 300, 300,
                     500, 500, 500, 500, 500,
                     643.8,
                     800, 800),
               rho = c(0.55126e2, 0.6e2, 0.65e2,
                       0.5e-1, 0.5, 0.4626e2, 0.5e2, 0.6e2,
                       0.2e2,
                       0.1e-1, 0.25) * M)
tab[, c("cv", "s")] <- tab[, c("cv", "s")] / M
format(tab, scientific = TRUE, digits = 9)
# Viscosity Tab. 3
tab <- heavy17("eta", t = c(298.15, 298.15, 298.15, 373.15,
                            775.0, 775.0, 775.0),
               rho = c(0, 1105, 1130, 1064, 1, 100, 400))
```

heavy17_sat

heavy17_sat

IAPWS-17 Formulation in the Saturation Region

Description

Compute thermodynamic and transport properties of heavy water along the saturated line according to the IAPWS formulation 2017.

Usage

```
heavy17_sat(what, p, t)
```

Arguments

what a character vector listing the output properties. See Details for available properties.

t a numeric vector giving the temperature values in K.

p a numeric vector giving the pressure values in MPa.

Details

- "f": the specific free energy in kJ/kg.
- "g": the specific Gibbs enthalpy in kJ/kg.
- "u": the specific internal energy in kJ/kg.
- "h": the specific enthalpy in kJ/kg.
- "s": the specific entropy in kJ/K/kg.

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- "t": the temperature in K.
- "p": the pressure in MPa.
- "v": the specific volume in m³/kg.
- "rho": the mass density in kg/m³.
- "cv": the specific isochoric heat capacity in kJ/K/kg.
- "cp": the specific isobaric heat capacity in kJ/K/kg.
- "alpha": the expansion coefficient in 1/K
- "beta": the pressure coefficient in MPa/K.
- "kappat": the isothermal compressibility in 1/MPa.
- "w": the speed of sound in m/s.
- "eta": the dynamic viscosity in μ Pa.s.
- "lambda": the thermal conductivity in mW/K/m.

Only one of t or p is needed. If both arguments are given, p is ignored.

Value

A numeric array of dimension c(n, length(what), 2L) with n the length of either p or t. The last dimension indicate the physical state ("liquid" or "gas").

Note

Computing several properties in a single call may be more efficient than separately because most of the computation time is shared.

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R16-17(2018), Revised Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water.

```
# IAPWS-17 Tab. 8
M <- 20.027508  # g/mol
tab <- heavy17_sat(c("p", "rho", "h", "s"), t = c(280, 450, 625))
format(tab, scientific = TRUE, digits = 9)</pre>
```

heavy17_state

heavy17_state

IAPWS-17 Physical States

Description

Identify the physical state of heavy water according to the IAPWS formulation 2017.

Usage

```
heavy17_state(p, t, rho)
```

Arguments

a numeric vector giving the pressure values in MPa.
 a numeric vector giving the temperature values in K.
 a numeric vector giving the density values in kg/m³.

Details

A valid pair of p, rho, t is needed: either (p, t) or (rho, t).

Value

A character vector giving the physical state. One of "solid", "liquid", "gas", "supercritical", "saturated" or "undef".

Author(s)

Jonathan Debove

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IAPWS

Constants built into iapws

Description

IAPWS and IAPWS95 contain constants relative to ordinary water substance. HEAVY17 is the same but for heavy water.

Usage

IAPWS IAPWS95 HEAVY17

Format

IAPWS, IAPWS95 and HEAVY17 are numeric verctors with with the following named elements:

```
"R" molar gas constant in J/K/mol.
```

"M" molar mass in g/mol.

"Pc" critical pressure in MPa.

"Tc" critical temperature in K.

"RHOc" critical density in kg/m³.

"Pt" triple-point pressure in MPa.

"Tt" triple-point temperature in K.

Examples

```
# Convert critical density of water in mol/L
IAPWS["RHOc"] / IAPWS["M"]
```

iapws95

IAPWS-95 Formulation in Single Phase Regions

Description

Compute thermodynamic and transport properties of water and steam using the IAPWS formulation 1995.

Usage

```
iapws95(what, p, t, rho, h, state = NULL)
```

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Arguments

what	a character vector listing the output properties. See Details for available properties.
р	a numeric vector giving the pressure values in MPa.
t	a numeric vector giving the temperature values in K.
rho	a numeric vector giving the density values in kg/m ³ .
h	a numeric vector giving the specific enthalpy values in kJ/kg.
state	NULL or a character vector giving the physical state. One of "liquid", "gas" or "supercritical". In case of NULL, the state is determined by the function iapws95_state().

Details

The available properties for what are:

- "f": the specific free energy in kJ/kg.
- "g": the specific Gibbs enthalpy in kJ/kg.
- "u": the specific internal energy in kJ/kg.
- "h": the specific enthalpy in kJ/kg.
- "s": the specific entropy in kJ/K/kg.
- "t": the temperature in K.
- "p": the pressure in MPa.
- "v": the specific volume in m³/kg.
- "rho": the mass density in kg/m³.
- "cv": the specific isochoric heat capacity in kJ/K/kg.
- "cp": the specific isobaric heat capacity in kJ/K/kg.
- "alpha": the expansion coefficient in 1/K
- "beta": the pressure coefficient in MPa/K.
- "kappat": the isothermal compressibility in 1/MPa.
- "w": the speed of sound in m/s.
- "eta": the dynamic viscosity in μ Pa.s.
- "lambda": the thermal conductivity in mW/K/m.

A valid pair of p, rho, t and h is needed: either (p, t), (rho, t) or (p, h).

Value

A numeric matrix of dimension c(n, length(what)) with n the maximum length of either rho, p, t, h or state.

Note

Computing several properties in a single call may be more efficient than separately because most of the computation time is shared.

iapws95

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R6-95(2018), Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use.

International Association for the Properties of Water and Steam, IAPWS R12-08(2008), *Release on the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance.*

International Association for the Properties of Water and Steam, IAPWS R15-11(2011), *Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance.*

```
# IAPWS-95 Tab. 7
tab <- iapws95(c("p", "cv", "w", "s"),
               t = c(300, 300, 300,
                     500, 500, 500, 500,
                     647,
                     900, 900, 900).
               rho = c(0.9965560e3, 0.1005308e4, 0.1188202e4,
                       0.4350000e0, 0.4532000e1, 0.8380250e3, 0.1084564e4,
                       0.3580000e3,
                       0.2410000e0, 0.5261500e2, 0.8707690e3))
format(tab, scientific = TRUE, digits = 9)
# Viscosity Tab. 4
tab <- iapws95("eta",
               t = c(298.15, 298.15, 373.15,
                     433.15, 433.15,
                     873.15, 873.15, 873.15,
                     1173.15, 1173.15, 1173.15),
               rho = c(998, 1200, 1000,
                       1, 1000,
                       1, 100, 600,
                       1, 100, 400))
format(tab, digits = 8)
# Viscosity Tab. 5
tab <- iapws95("eta", t = 647.35, rho = c(122, 222, 272, 322, 372, 422))
format(tab, digits = 8)
# Thermal conductivity Tab. 4
tab <- iapws95("lambda", t = c(298.15, 298.15, 298.15, 873.15),
               rho = c(0, 998, 1200, 0)
format(tab, digits = 9)
```

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iapws95_sat

IAPWS-95 Formulation in the Saturation Region

Description

Compute thermodynamic and transport properties of water and steam along the saturated line according to the IAPWS formulation 1995.

Usage

```
iapws95_sat(what, p, t)
```

Arguments

what	a character vector listing the output properties. See Details for available properties.
t	a numeric vector giving the temperature values in K.
р	a numeric vector giving the pressure values in MPa.

Details

- "f": the specific free energy in kJ/kg.
- "g": the specific Gibbs enthalpy in kJ/kg.
- "u": the specific internal energy in kJ/kg.
- "h": the specific enthalpy in kJ/kg.
- "s": the specific entropy in kJ/K/kg.
- "t": the temperature in K.
- "p": the pressure in MPa.
- "v": the specific volume in m³/kg.
- "rho": the mass density in kg/m³.
- "cv": the specific isochoric heat capacity in kJ/K/kg.
- "cp": the specific isobaric heat capacity in kJ/K/kg.
- "alpha": the expansion coefficient in 1/K
- "beta": the pressure coefficient in MPa/K.
- "kappat": the isothermal compressibility in 1/MPa.

iapws95_state

- "w": the speed of sound in m/s.
- "eta": the dynamic viscosity in μ Pa.s.
- "lambda": the thermal conductivity in mW/K/m.

Only one of t or p is needed. If both arguments are given, p is ignored.

Value

A numeric array of dimension c(n, length(what), 2L) with n the length of either p or t. The last dimension indicate the physical state ("liquid" or "gas").

Note

Computing several properties in a single call may be more efficient than separately because most of the computation time is shared.

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R6-95(2018), Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use.

Examples

```
# IAPWS-95 Tab. 8
tab <- iapws95_sat(c("p", "rho", "h", "s"), t = c(275, 450, 625))
format(tab, scientific = TRUE, digits = 9)</pre>
```

iapws95_state

IAPWS-95 Physical States

Description

Identify the physical state of water according to the IAPWS formulation 1995.

Usage

```
iapws95_state(p, t, rho)
```

Arguments

p a numeric vector giving the pressure values in MPa.
t a numeric vector giving the temperature values in K.
rho a numeric vector giving the density values in kg/m³.

iapws_epsilon

Details

```
A valid pair of p, rho, t is needed: either (p, t) or (rho, t).
```

Value

```
A character vector giving the physical state. One of "solid", "liquid", "gas", "supercritical", "saturated" or "undef".
```

Author(s)

Jonathan Debove

Examples

iapws_epsilon

IAPWS Formulations for Electrostatic Properties of Water

Description

Compute the dielectric constant, refractive index and ionization constant of water.

Usage

```
iapws_epsilon(rho, t)
iapws_n(rho, t, lambda)
iapws_pk(rho, t)
```

Arguments

rho a numeric vector giving the density values in kg/m³. t a numeric vector giving the temperature values in K. lambda a numeric vector giving the wavelenth values in μ m.

Details

For calculating the properties as function of pressure, the function iapws95() should be employed.

Value

A numeric vector.

Author(s)

Jonathan Debove

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References

International Association for the Properties of Water and Steam, IAPWS R8-97, Release on the Static Dielectric Constant of Ordinary Water Substance for Temperatures from 238 K to 873 K and Pressures up to 1000 MPa.

International Association for the Properties of Water and Steam, IAPWS R9-97, Release on the Refractive Index of Ordinary Water Substance as Function of Wavelength, Temperature and Pressure.

International Association for the Properties of Water and Steam, IAPWS R11-07(2019), *Revised Release on the Ionization Constant of H2O*.

Examples

```
# Dielectric constant Tab. 4
t <- c(240, 300, 300, 300, 650, 650, 650, 870, 870, 870)
rho <- iapws95("rho", t = t,
               p = c(0.1013125, 0.1013125, 10, 1000,
                      10, 100, 500, 10, 100, 500),
               state = c(rep("liquid", 4),
                          "gas", rep("supercritical", 2),
                          "gas", rep("supercritical", 2)))
tab <- iapws_epsilon(rho, t)</pre>
print(tab, digits = 6)
# Refractive index Tab. 3
d \leftarrow expand.grid(t = c(0, 100, 200, 500) + 273.15,
p = c(0.1, 1, 10, 100),
                 lambda = c(0.2265, 0.589, 1.01398))
dstate <- iapws95_state(p = d$p, t = d$t)
d$state[d$state == "solid"] <- "liquid"
d$rho \leftarrow drop(iapws95("rho", t = d$t, p = d$p, state = d$state))
tab <- iapws_n(d$rho, d$t, d$lambda)</pre>
dim(tab) <- c(4, 4, 3)
print(tab, digits = 8)
# Ionization constant Tab. 3
tab <- iapws_pk(rho = c(1, 0.07, 0.7, 0.2, 1.2) * 1e3,
                t = c(300, 600, 600, 800, 800))
print(tab, digits = 7)
```

 ${\tt iapws_sigma}$

IAPWS Formulations for Surface Tension

Description

Compute the surface tension of ordinary and heavy water.

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Usage

```
iapws_sigma(t)
heavy17_sigma(t)
```

Arguments

t a numeric vector giving the temperature values in K.

Value

A numeric vector giving the values of surface tension in mN/m.

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R1-76(2014), Revised Release on Surface Tension of Ordinary Water Substance.

International Association for the Properties of Water and Steam, IAPWS R5-85(1994), IAPWS Release on Surface Tension of Heavy Water Substance.

Examples

```
print(iapws\_sigma(seq(5, 370, by = 5) + 273.15), digits = 2)
print(heavy17\_sigma(seq(5, 370, by = 5) + 273.15), digits = 1)
```

ice06

Equation of State 2006 for Ice Ih

Description

Compute thermodynamic properties of ice Ih using the Equation of State 2006.

Usage

```
ice06(what, p, t)
```

Arguments

what a character vector listing the output properties. See Details for available properties.

p a numeric vector giving the pressure values in MPa.

t a numeric vector giving the temperature values in K.

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Details

The available properties for what are:

- "f": the specific free energy in kJ/kg.
- "g": the specific Gibbs enthalpy in kJ/kg.
- "u": the specific internal energy in kJ/kg.
- "h": the specific enthalpy in kJ/kg.
- "s": the specific entropy in kJ/K/kg.
- "t": the temperature in K.
- "p": the pressure in MPa.
- "v": the specific volume in m³/kg.
- "rho": the mass density in kg/m³.
- "cv": the specific isochoric heat capacity in kJ/K/kg.
- "cp": the specific isobaric heat capacity in kJ/K/kg.
- "alpha": the expansion coefficient in 1/K
- "beta": the pressure coefficient in MPa/K.
- "kappat": the isothermal compressibility in 1/MPa.
- "w": the speed of sound in m/s.

Value

A numeric matrix of dimension c(n, length(what)) with n the maximum length of either p or t.

Note

Computing several properties in a single call may be more efficient than separately because most of the computation time is shared.

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R10-06(2009), *Revised Release on the Equation of State 2006 for H2O Ice Ih.*

```
tab <- ice06(c("g", "h", "f", "u", "s", "cp", "rho", "alpha", "beta", "kappat"), p = c(611.657e-6, .101325, 100), t = c(273.16, 273.152519, 100)) format(tab, scientific = TRUE, digits = 11)
```

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if97

IAPWS-IF97 Equations for Regions 1, 2, 3 and 5

Description

Compute thermodynamic and transport properties of water and steam using the IAPWS industrial formulation 1997.

Usage

```
if97(what, p, t, h, state = NULL)
```

Arguments

what	a character vector listing the output properties. See Details for available properties.
р	a numeric vector giving the pressure values in MPa.
t	a numeric vector giving the temperature values in K.
h	a numeric vector giving the specific enthalpy values in kJ/kg.
state	NULL or a character vector giving the physical state. One of "liquid", "gas" or "supercritical". In case of NULL, the state is determined by the function if97_state().

Details

- "f": the specific free energy in kJ/kg.
- "g": the specific Gibbs enthalpy in kJ/kg.
- "u": the specific internal energy in kJ/kg.
- "h": the specific enthalpy in kJ/kg.
- "s": the specific entropy in kJ/K/kg.
- "t": the temperature in K.
- "p": the pressure in MPa.
- "v": the specific volume in m³/kg.
- "rho": the mass density in kg/m³.
- "cv": the specific isochoric heat capacity in kJ/K/kg.
- "cp": the specific isobaric heat capacity in kJ/K/kg.
- "alpha": the expansion coefficient in 1/K
- "beta": the pressure coefficient in MPa/K.
- "kappat": the isothermal compressibility in 1/MPa.
- "w": the speed of sound in m/s.

if97

- "eta": the dynamic viscosity in μ Pa.s.
- "lambda": the thermal conductivity in mW/K/m.

A valid pair of p, t and h is needed: either (p, t) or (p, h).

Value

A numeric matrix of dimension c(n, length(what)) with n the maximum length of either p, t, h or state.

Note

Computing several properties in a single call may be more efficient than separately because most of the computation time is shared.

Author(s)

Jonathan Debove

References

International Association for the Properties of Water and Steam, IAPWS R7-97(2012), Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam.

International Association for the Properties of Water and Steam, IAPWS R12-08(2008), *Release on the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance.*

International Association for the Properties of Water and Steam, IAPWS R15-11(2011), *Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance.*

if97_sat

if97_sat

IAPWS-IF97 Equations in Region 4

Description

Compute the pressure and the temperature along the saturated line according to the IAPWS industrial formulation 1997.

Usage

```
if97_psat(t)
if97_tsat(p)
```

Arguments

t a numeric vector giving the temperature values in K.

p a numeric vector giving the pressure values in MPa.

Value

A numeric vector containing the saturation-pressure (MPa) or the saturation-temperature (K). Return NA for inputs outside of the range of validity.

Author(s)

Jonathan Debove

if97_state

References

International Association for the Properties of Water and Steam, IAPWS R7-97(2012), Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam.

Examples

```
# Region 4 format(if97_psat(t = c(300, 500, 600)), scientific = TRUE, digits = 9) format(if97_tsat(p = c(0.1, 1.0, 10.0)), scientific = TRUE, digits = 9)
```

if97_state

IAPWS-IF97 Physical States

Description

Identify the physical state of water according to the IAPWS industrial formulation 1997.

Usage

```
if97_state(p, t)
```

Arguments

p a numeric vector giving the pressure values in MPa.t a numeric vector giving the temperature values in K.

Value

A character vector giving the physical state. One of "solid", "liquid", "gas", "supercritical", "saturated" or "undef".

Author(s)

Jonathan Debove

```
if97\_state(p = c(.1, .1, 23), t = c(293.15, 373.15, 650))
```

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