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Description Calculation of gas transport properties (viscosity, diffusion, thermal conductivity) using Chapman-Enskok theory (Chapman 1918, <doi:10.1098/rsta.1918.0005>) and of the second virial coefficient (Vargas et al. 2001, <doi:10.1016/s0378-4371(00)00362-9>) using the Lennard-Jones (12-6) potential. Up to the third order correction is taken into account for viscosity and thermal conductivity. It is also possible to calculate the binary diffusion coefficients of polar and non-polar gases in non-polar bath gases (Brown et al. 2011, <doi:10.1016/j.pecs.2010.12.001>). 16 collision integrals are calculated with four digit accuracy over the reduced temperature range [0.3, 400] using an interpolation function of Kim and Monroe (2014, <doi:10.1016/j.jcp.2014.05.018>).

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chapensk-package *Estimation of Gas Properties from the Lennard-Jones Potential*

Description

Calculation of gas transport properties (viscosity, diffusion, thermal conductivity) using Chapman-Enskok theory (Chapman 1918, <doi:10.1098/rsta.1918.0005>) and of the second virial coefficient (Vargas et al. 2001, <doi:10.1016/s0378-4371(00)00362-9>) using the Lennard-Jones (12-6) potential. Up to the third order correction is taken into account for viscosity and thermal conductivity. It is also possible to calculate the binary diffusion coefficients of polar and non-polar gases in non-polar bath gases (Brown et al. 2011, <doi:10.1016/j.pecs.2010.12.001>). 16 collision integrals are calculated with four digit accuracy over the reduced temperature range [0.3, 400] using an interpolation function of Kim and Monroe (2014, <doi:10.1016/j.jcp.2014.05.018>).

Introduction

Transport properties, such as viscosity, diffusion and thermal conductivity, play a crucial role in the modeling of combustion processes and chemical reactions. They depend on the intermolecular potential. In practice it is not necessary to have a detailed calculation of the intermolecular potential for the calculation of transport properties.

The interaction between spherical gas particles without a dipole moment can be described by the Lennard-Jones potential. It is given by the following equation:

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

where r is the distance between two interacting particles, ε is the depth of the potential well and σ is the distance at which the particle-particle potential energy U is zero. The theory of van der Waals interaction gives the exponent 6 for the attractive term (London, 1937). The 12 exponent in the repulsive term is largely a matter of computational practicality, though it does represent the general nature of Pauli repulsion.

The Lennard-Jones potential only can be used for non-polar molecules, but sometimes is also used for polar molecules. However, for the latter the Stockmayer (12-6-3) potential is more appropriate (Mourits and Rummens, 1977).

For monoatomic gases σ and ε are independent of temperature. However, for non-monoatomic gases, averaging over different orientations and vibrational states gives temperature dependent parameters σ and ε (Zarkova and Hohm, 2002). The temperature dependency is simplified in this package as follows by a linear temperature coefficient ζ:

$$\sigma(T) = \sigma + \zeta T$$

$$\varepsilon(T) = \varepsilon \left(\frac{\sigma}{\sigma + \zeta T} \right)^6$$

The Chapman-Enskog theory is a theoretical framework used to describe the transport properties of gases, such as viscosity, thermal conductivity, and diffusion coefficients. The theory is based on the idea that the properties of a gas can be related to the collisional interactions between individual gas molecules (Chapman 1918).

Collision integrals are mathematical expressions that arise in the Chapman-Enskog theory. They quantify the effects of molecular collisions on the transport properties of a gas.

Methods

An object-oriented framework has been developed to calculate transport properties from potential parameters and vice versa. A class Gas has been defined for the calculation of the properties of gas. To facilitate calculations, a data set gas is provided for the properties of some common gases. The CollisionIntegral class is used to calculate collision integrals using an interpolation function and fit parameters from data set coefficients_collisionintegral.

Results

Lennard-Jones parameters of non-polar molecules can be estimated using high quality of viscosity and second virial coefficients. This is demonstrated for ethane, see data set ethane_data. For polar molecules Lennard-Jones parameters for the van der Waals interaction part can be estimated from measurements of binary diffusion coefficients, see data set binary_diffusion.

Nomenclature

Symbol	Description	Unit	Global variable
b	temperature coefficient of diffusion	-	
B	second virial coefficient	m3	
D	diffusion coefficient	m2/2	
k	Boltzmann constant	J/K	pkg.env$k
m	molecular mass	kg	
M	relative molecular mass	-	
N_a	Avogadro constant	1/mol	pkg.env$Na
n	mole	mol	
p	pressure	Pa	
p_0	standard pressure 101325 Pa	Pa	pkg.env$p0
p_c	critical pressure	Pa	
R	gas constant	J/(K.mol)	pkg.env$R
T	temperature	K	
T_0	standard temperature 273.15 K	K	pkg.env$T0
T_c	critical temperature	K	
V	gas volume	m3	
α	polarizability	Ao3	
$\bar{\alpha}$	reduced polarizability	-	
η	dynamic viscosity	Pa.s	
ϵ	permittivity of vacuum	F/m	pkg.env$eps0

ε	depth of potential well	J
κ	thermal conductivity	W/(m.K)
μ	dipole moment	D
$\bar{\mu}$	reduced dipole moment	-
Ω	reduced collision integral	-
ρ	gas density	kg/m3
ρ_c	critical density	mol/l
Θ	reduced temperature	-
σ	distance at which the potential energy is zero	Ao
ξ	scaling parameter	-
ζ	temperature coefficient of σ	Ao/K

Physical units are displayed in UCUM notation.

Author(s)

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Maintainer: Stefan Langenberg <langenberg@uni-bonn.de>

References

Brown NJ, Bastien LAJ, Price PN. Transport properties for combustion modeling. *Progress in Energy and Combustion Science* 2011;37:565-82. doi:10.1016/j.pecs.2010.12.001.

Chapman SV. On the kinetic theory of a gas. Part II. A composite monatomic gas: diffusion, viscosity, and thermal conduction. *Philosophical Transactions of the Royal Society of London. Series A* 1918;217:11597. doi:10.1098/rsta.1918.0005.

London F. The general theory of molecular forces. *Transactions of the Faraday Society* 1937;33:8b. doi:10.1039/tf937330008b.

Mourits FM, Rummens FHA. A critical evaluation of Lennard-Jones and Stockmayer potential parameters and of some correlation methods. *Can. J. Chem.* 1977;55:300720. doi:10.1139/v77-418.

Zarkova L, Hohm U. pVT-Second Virial Coefficients $B(T)$, Viscosity η and Self-Diffusion $\rho D(T)$ of the Gases: BF3, CF4, SiF4, CCl4, SiCl4, SF6, MoF6, WF6, UF6, C(CH3)4, and Si(CH3)4 Determined by Means of an Isotropic Temperature-Dependent Potential. *Journal of Physical and Chemical Reference Data* 2002;31:183216. doi:10.1063/1.1433462.

`binary_diffusion` *Binary gas phase diffusion coefficients of methane, ethane, propane and butane in helium and nitrogen; fluoromethane, difluoromethane and trifluoromethane in nitrogen; sulfur dioxide in hydrogen, helium and nitrogen measured by reverse-flow gas chromatography*

Description

Reference data of binary diffusion coefficients for comparison with calculated diffusion coefficients. Diffusion coefficients were determined using a reversed-flow gas chromatography system.

Usage

```
data("binary_diffusion")
```

Format

A data frame with 139 observations on the following 6 variables.

`doi` DOI of data source

`bath_gas` Bath gas: helium, hydrogen, nitrogen

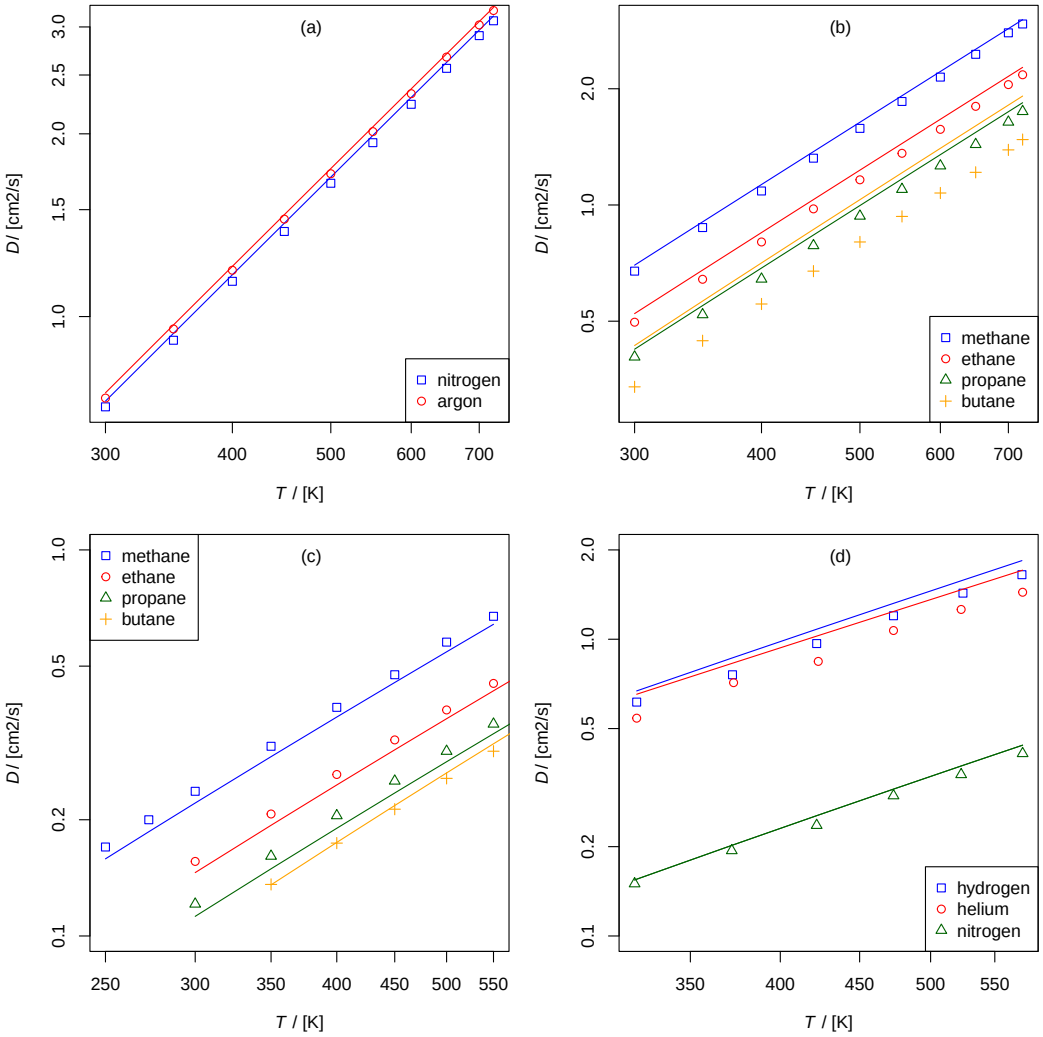
`gas` Diffusing species: argon, butane, difluoromethane, ethane, fluoromethane, methane, nitrogen, propane, sulfur dioxide, trifluoromethane

`T` Temperature in `K`

`D` Diffusion coefficient in `cm2/s`

`U_D` Uncertainty of diffusion coefficient in `cm2/s`

Details



Plot of experimental diffusion coefficient vs. temperature. (a) diffusion of nitrogen and argon in helium. (b) diffusion of methane, ethane, propane and butane in helium. (c) diffusion of methane, ethane, propane and butane in nitrogen. (d) diffusion of sulfur dioxide in hydrogen, helium and nitrogen. The solid lines are calculated using the Lennard-Jones model. The Lennard-Jones parameters are taken from data set gas.

The diffusion coefficient D as function of pressure in a narrow temperature range close to the reference temperature T_0 is usually expressed as (Langenberg *et al.* 2020)

$$D = D_0 \left(\frac{p_0}{p}\right) \left(\frac{T}{T_0}\right)^b$$

For the experimental data, the temperature coefficient b is obtained from the fit. For the calculated

diffusion coefficients, the temperature coefficient is calculated by numerical derivation by

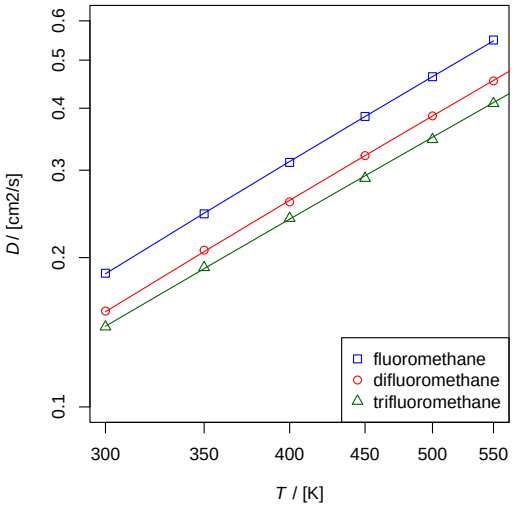
$$b = \left(\frac{\partial D}{\partial T}\right)_{T_0} \left(\frac{T_0}{D_0}\right).$$

The diffusion coefficients D_{calc} are calculated using Gas-class. The deviation is calculated by

$$\frac{D_{\mathrm{exp}} - D_{\mathrm{calc}}}{D_{\mathrm{exp}}}.$$

Gas	Bath gas	Experimental		Calculated		Deviation
		D_0 / [cm2/s]	b	D_0 / [cm2/s]	b	
nitrogen	helium	0.605(3)	1.664(8)	0.620	1.68	-3%
argon	helium	0.630(2)	1.665(6)	0.640	1.68	-2%
methane	helium	0.575(3)	1.675(7)	0.597	1.68	-4%
ethane	helium	0.421(5)	1.68(2)	0.446	1.70	-6%
propane	helium	0.341(7)	1.67(2)	0.361	1.70	-7%
n-butane	helium	0.294(6)	1.65(2)	0.368	1.74	-32%
methane	nitrogen	0.201(2)	1.74(2)	0.186	1.83	7%
ethane	nitrogen	0.136(2)	1.70(2)	0.123	1.87	7%
propane	nitrogen	0.106(2)	1.72(3)	0.094	1.88	7%
n-butane	nitrogen	0.090(1)	1.72(2)	0.084	1.97	-8%
sulfur dioxide	hydrogen	0.45(2)	1.77(6)	0.492	1.85	-14%
sulfur dioxide	helium	0.41(2)	1.7(1)	0.490	1.71	-14%
sulfur dioxide	nitrogen	0.112(3)	1.76(5)	0.113	1.91	-8%

The values in brackets indicate the uncertainties (0.95 confidence level) of the fit parameters. With the exception of the diffusion of butane in helium, the calculated diffusion coefficients resemble the measured diffusion coefficients within an error limit of < 15%. For larger non spherical molecules like butane in helium more advanced combining rules need to be applied (Li *et al.* 2023).



Plot of experimental diffusion coefficient vs. temperature of fluoromethane, difluoromethane and

trifluoromethane in nitrogen. The Lennard-Jones parameters are estimated by nonlinear regression using optim from experimental data.

The experimental data for the diffusion coefficients of fluoromethanes can in turn be used to estimate the Lennard-Jones parameters for the Van der Waals interaction. The values for ε obtained from diffusion data are smaller than ε obtained from data of viscosity measurements (Shibasaki-Kitakawa *et. al.* 1995, Clifford *et al.* 1979).

Gas	D_0/ [cm2/s]	b	Viscosity		Diffusion	
			σ / [Ao]	ε/k / [K]	σ / [Ao]	ε/k / [K]
fluoromethane	0.1576(7)	1.784(8)	–	–	3.5	174
difluoromethane	0.133(2)	1.76(2)	4.9	204	3.9	153
trifluoromethane	0.123(2)	1.73(2)	4.4	182	4.5	63

This is due to the fact that the fluoromethanes have a dipole moment. Thus, the well depth of the potential is higher, compared to the only van der Waals interaction. This is why the intermolecular interaction of polar molecules cannot be described in terms of the Lennard-Jones potential.

Source

McGivern WS, Manion JA. Extending reversed-flow chromatographic methods for the measurement of diffusion coefficients to higher temperatures. *J. Chromatogr. A* 2011; 1218:8432-42. doi:10.1016/j.chroma.2011.09.035.

McGivern WS, Manion JA. Hydrocarbon binary diffusion coefficient measurements for use in combustion modeling. *Combustion and Flame* 2012;159:3021-6. doi:10.1016/j.combustflame.2012.04.015.

McGivern WS, Manion J. Binary Diffusion Coefficients for Methane and Fluoromethanes in Nitrogen. *Journal of Chemical & Engineering Data* 2021; 66:304756. doi:10.1021/acs.jced.1c00161.

Tsaousoglou DP, Georgiadou E, Gavril D. Determination of Sulfur Dioxide Diffusion Coefficients in Hydrogen, Helium, and Nitrogen by Reversed-Flow Inverse Gas Chromatography. *J. Chem. Eng. Data* 2022; 67:28728. doi:10.1021/acs.jced.2c00223.

References

Clifford AA, Gray P, Scott AC. Viscosities of CFCl3, CF3Cl, CHFCl2, CHF2Cl and CHF3 from 373 to 570 K. *J. Chem. Soc., Faraday Trans. 1*, 1979;75:1752. doi:10.1039/F19797501752

Langenberg S, Carstens T, Hupperich D, Schweighoefer S, Schurath U. Technical note: Determination of binary gas-phase diffusion coefficients of unstable and adsorbing atmospheric trace gases at low temperature arrested flow and twin tube method. *Atmospheric Chemistry and Physics* 2020;20:366982. doi:10.5194/acp2036692020.

Li Y, Gui Y, You X. On the binary diffusion coefficients of n-alkanes in He/N2. *Combustion and Flame* 2023;257:112795. doi:10.1016/j.combustflame.2023.112795.

Shibasaki-Kitakawa N, Takahashi M, Yokoyama C, Takahashi S. Gas Viscosity of Difluoromethane from 298.15 to 423.15 K and up to 10 MPa *J. Chem. Eng. Data* 1995; 40:900-902 doi:10.1021/je00020a036

Examples

```
# binary diffusion data of nitrogen in bath gas helium
nitrogen_in_helium <- subset(binary_diffusion,(gas=="nitrogen" & bath_gas=="helium"))
print(nitrogen_in_helium)
```

`coefficients_collisionintegral` *Coefficients to calculate collision integrals for the Lennard Jones (12-6) potential*

Description

Coefficients for "CollisionIntegral", Table 1 from Kim and Monroe (2014).

Usage

```
data("coefficients_collisionintegral")
```

Format

`l` order of collision integral s

`s` order of collision integral l

`A` model parameter A

`B1` model parameter B_1

`B2` model parameter B_2

`B3` model parameter $B_3 \times 10$

`B4` model parameter $B_4 \times 10$

`B5` model parameter $B_5 \times 100$

`B6` model parameter $B_6 \times 1000$

`C1` model parameter C_1

`C2` model parameter $C_2 \times 10$

`C3` model parameter $C_3 \times 10$

`C4` model parameter $C_4 \times 100$

`C5` model parameter $C_5 \times 1000$

`C6` model parameter $C_6 \times 10000$

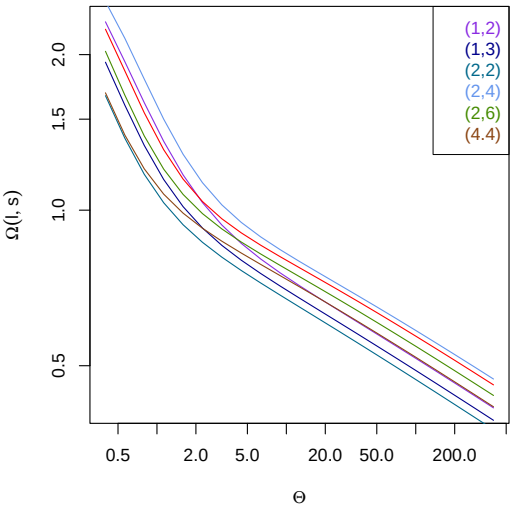
Source

Kim SU, Monroe CW. High-accuracy calculations of sixteen collision integrals for Lennard-Jones (12-6) gases and their interpolation to parameterize neon, argon, and krypton. *Journal of Computational Physics* 2014;273:35873. doi:10.1016/j.jcp.2014.05.018.

`CollisionIntegral-class` *Class* `"CollisionIntegral"`

Description

Class for the empirical interpolation functions for 16 reduced Lennard-Jones (12-6) collision integrals in the range 0.3 <= Θ <= 400.



Collision integrals as function of reduced temperature Θ

Fields

`l`: order of collision integral l

`s`: order of collision integral s

`coeff`: coefficients for collision integrals for order l and s, see data set `coefficients_collisionintegral`

`A`: model parameter A

`B`: model parameter B_1 ... B_6

`C`: model parameter C_1 ... C_6

Methods

`initialize(s, l)`: Initialize reduced collision integral of order l and s

`Omega(Theta)`: Calculates reduced collision integral Ω(l,s) at reduced temperature Θ using the empirical interpolation function

$$\Omega^{(l,s)} = A^{(l,s)} + \sum_{k=1}^{6} \left[\frac{B_k^{(l,s)}}{\Theta^k} + C_k^{(l,s)} (\ln \Theta)^k \right]$$

References

Kim SU, Monroe CW. High-accuracy calculations of sixteen collision integrals for Lennard-Jones (12-6) gases and their interpolation to parameterize neon, argon, and krypton. *Journal of Computational Physics* 2014;273:35873. doi:10.1016/j.jcp.2014.05.018.

Examples

```
O11 <- CollisionIntegral(l=1,s=1)
O11$Omega(0.3)
```

`ethane_data` *Viscosity and second virial coefficient of ethane*

Description

Reference values for the second virial coefficient and viscosity of ethane from a intermolecular potential energy surface. The second virial coefficient was calculated semiclassically by means of the Mayer-sampling Monte Carlo technique, while the transport properties were obtained using the classical kinetic theory of polyatomic gases. The computed thermophysical property values are in excellent agreement with the best available experimental data and are recommended as reference values.

Usage

```
data("ethane_data")
```

Format

A data frame with 107 observations on the following 4 variables.

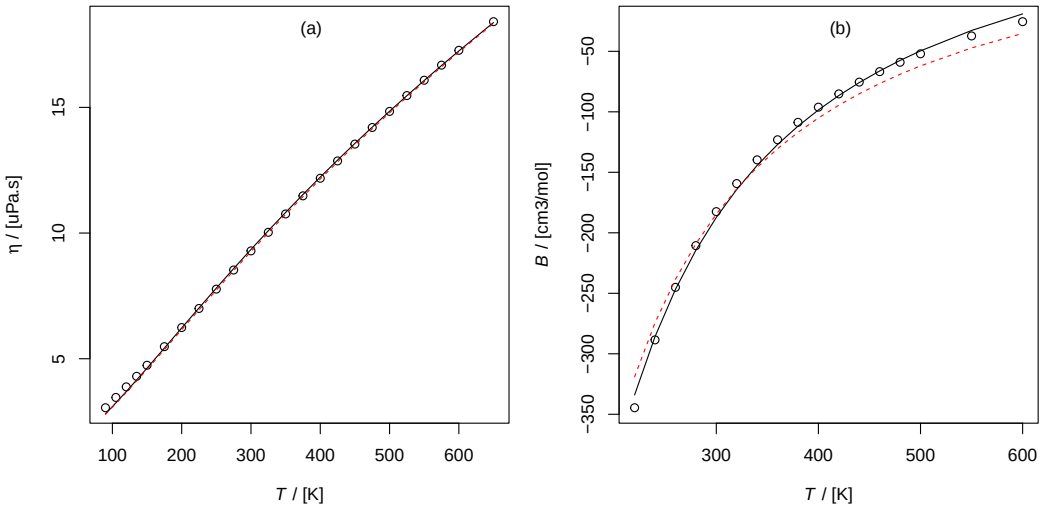
`T` Temperature in `K`

`property` Type of property. `B`: classically calculated second virial coefficient, `BQFH`: second virial coefficient calculated by a modification of the pair potential known as the quadratic Feynman-Hibbs (QFH) effective pair potential. `viscosity`: gas phase viscosity

`unit` a factor with levels `cm3/mol`, `uPa.s`

`value` numerical value of property. For the second virial coefficient the calculated data are supported by experimental data in the temperature range 220 - 623 K. For the viscosity the calculated data are supported by experimental data in the temperature range 90 - 675 K.

Details



(a) Viscosity of ethane. (b) second virial coefficient of ethane. The black solid curves are fits using viscosity data and second virial coefficient data respectively. The red dotted curves are simultaneous fits against the viscosity and second virial coefficient data.

Type of fit	σ	ε/k
vs. viscosity data	4.38(2)	235(6)
vs. second virial coefficient data	4.95(6)	202(3)
vs. viscosity and second virial coefficient data	4.35	244

Source

Hellmann R. Reference Values for the Second Virial Coefficient and Three Dilute Gas Transport Properties of Ethane from a State-of-the-Art Intermolecular Potential Energy Surface. *Journal of Chemical & Engineering Data* 2018;63:470-81. doi:10.1021/acs.jced.7b01069.

Examples

```
## Not run:
c2h6 <- Gas("ethane")
# estimate LJ-coefficients from viscosity data
ethane_viscosity <- subset(ethane_data,
  (property=="viscosity") & (T>=90) & (T<=675), select=c(T, value)
)
c2h6$dsigma_dt <- 0
ethane_viscosity$value <- 1E-6*ethane_viscosity$value
c2h6$fit_viscosity_data(ethane_viscosity)
print(c2h6$sigma)
print(c2h6$epsk)

# estimate LJ-coefficients from second virial coefficient
ethane_B <- subset(ethane_data, (property=="BQFH") & (T>= 220) & (T<=623))
```

```
ethane_B$value <- 1E-6*ethane_B$value
c2h6$fit_B_data(ethane_B)
print(c2h6$sigma)
print(c2h6$epsk)

## End(Not run)
```

---

gas *Gas data*

Description

Physical properties of some gas species.

Usage

```
data("gas")
```

Format

A data frame with properties of 47 gases on the following 12 variables.

`formula` chemical formula

`name` chemical name

`CAS` Chemical abstracts registry number

`group` point group

`M` relative molecular mass

`dipole_moment` electric dipole moment in `Debye`

`polarizability` electric polarizability in `Ao`

`IE` ionization energy in `eV`

`Tc` critical temperature in `K`

`pc` critical pressure in `bar`

`rhoc` critical density in `mol/l`

`sigma` distance at which the intermolecular potential between the two particles is zero in `Ao`

`epsk` Well depth ε/k of the Lennard-Jones potential in `K`

`DOI` Data source of Lennard-Jones parameters. If not specified otherwise, they are taken from Poling *et al.* (2004)

Details

Properties of simple gases for the calculation of transport properties. Not all properties are given for all molecules.

Correlations exists between the Lennard-Jones parameters and critical data as derived from numerous numerical simulations of the Lennard-Jones fluid (Stephan *et al.* 2019): ε and σ can be determined from critical temperature

$$T_c = (1.321 \pm 0.007)(\varepsilon/k)$$

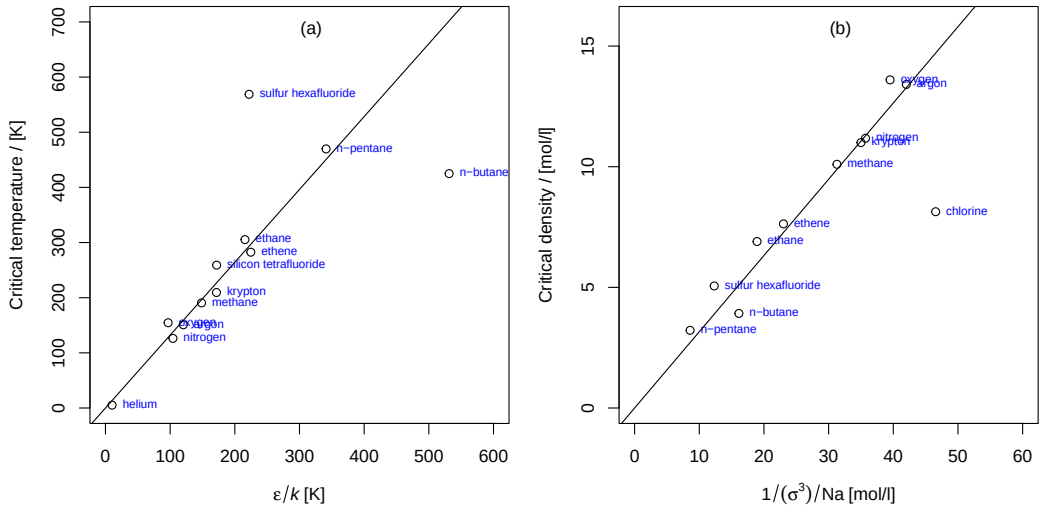
critical density

$$\rho_c = (0.316 \pm 0.005)/\sigma^3$$

and critical pressure

$$p_c = (0.129 \pm 0.005)(\varepsilon/\sigma^3)$$

where k is the Boltzmann constant.



Correlation of Lennard-Jones parameters of nonpolar gases with critical data: The solid lines are the expectations from numerical simulations of the Lennard-Jones Fluid. (a) critical temperature vs. well depth ε. (b) critical density vs. $1/\sigma^3$.

References

NIST Chemistry WebBook. NIST Standard Reference Database, vol. 69, 2023. doi:10.18434/T4D303.

NIST. Experimental Polarizabilites. in: III RDJ, editor. NIST Computational Chemistry Comparison and Benchmark Database, NIST; 2020. doi:10.18434/T47C7Z.

Poling BE, Prausnitz JM, OConnell JP. The Properties of Gases and Liquids. 5 ed. New York: McGraw-Hill; 2004.

Stephan S, Thol M, Vrabec J, Hasse H. Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. *Journal of Chemical Information and Modeling* 2019;59:424865. doi:10.1021/acs.jcim.9b00620.

Gas-class *Class* "Gas"

Description

Reference class for gas with methods for the estimation of transport properties. The equations for the higher order corrections are taken from Kim and Monroe 2014. The second virial coefficient is calculated using the equation given by Vargas *et al.* 2001.

Fields

`name`: Chemical name

`M`: relative molecular mass M

`m`: Mass m of one gas particle in `kg`

`sigma`: Lennard-Jones Parameter σ at $T = 0$

`zeta`: Change of σ with temperature. For the noble gases $\zeta = 0$. Due to the vibrational excitation of molecules, σ is not independent of temperature but increasing with T. If σ_0 is σ at $T = 0$, σ at T is given by $\sigma = \sigma_0 + \zeta T$.

`epsk`: Well depth of the Lennard-Jones potential ε/k at $T = 0$ in `K`.

`dipole_moment`: dipole moment μ in `Debye`.

`polarizability`: polarizability α in `Ao3`.

Methods

`check()`: Checks for presence of required data.

`B(T)`: Second virial coefficient $B(T)$ in units `m3/mol`. The second virial coefficient provides systematic corrections to the ideal gas law.

$$\frac{pV}{nRT} = 1 + \frac{n}{V}B + \ldots$$

The second virial coefficient B depends only on the pair interaction between the particles (Vargas et. al. 2001). It is calculated from the modified Bessel function I (BesselI):

$$B(\Theta) = \frac{\sqrt{2}\pi^2\sigma^3}{3\Theta}\left[I_{-3/4}\left(\frac{1}{2\Theta}\right) + I_{3/4}\left(\frac{1}{2\Theta}\right) - I_{1/4}\left(\frac{1}{2\Theta}\right) - I_{-1/4}\left(\frac{1}{2\Theta}\right)\right]$$

`density(p=p0,T=T0)`: Gas density in units `kg/m3` incorporating the second virial correction.

$$\rho = \frac{M}{2B(\Theta)}\left(\sqrt{1 + \frac{4pB(\Theta)}{RT}} - 1\right)$$

`diffusion(p=p0, T=T0, second_order_correction=TRUE)`: Calculates the self diffusion coefficient in `m2/s`.

$$D = \frac{3\sqrt{\pi m k T}}{8\pi\sigma^2\rho(p,T)\Omega^{(1,1)}(\Theta)} f_D^{(n)}$$

$f_D^{(n)}$ is the second order correction term. If `third_order_correction=FALSE` this term is set to 1.

`thermal_conductivity(T, third_order_correction=TRUE)`**:** Calculates the thermal conductivity for a monoatomic gas in `W/(m.K)`.

$$\kappa = \frac{75k}{64\sigma^2\Omega^{(2,2)}(\Theta)}\sqrt{\frac{kT}{\pi m}} f_\kappa^{(n)}$$

$f_\kappa^{(n)}$ is the third order correction term. If `third_order_correction=FALSE` this term is set to 1. For a polyatomic gas the thermal conductivity can be calculated from the expression for a monoatomic gas using the classical Eucken correction (Bechtel *et al.* 2020)

$$\kappa_p = \kappa\left(\frac{4c_v}{15R} + \frac{3}{5}\right)$$

where c_v is the molar heat capacity of the polyatomic gas at constant volume.

`viscosity(T,third_order_correction=TRUE)`**:** The viscosity η is given gas as

$$\eta = \frac{5\sqrt{\pi m T}}{16\pi\sigma^2\Omega^{(2,2)}(\Theta)} f_\eta^{(n)}.$$

$f_\eta^{(n)}$ is the third order correction term. If `third_order_correction=FALSE` this term is set to 1.

`binary_diffusion(p=p0, T=T0, bathGas)`**:** Binary Diffusion coefficient of gas 1 in a bath gas 2 `bathGas`. The gas 1 may be polar or nonpolar. The bath gas 2 must be nonpolar (Brown *et al.* 2010, Langenberg *et al.* 2020).

The binary diffusion coefficient D_{12} is given as

$$D_{12} = \frac{3}{16}\sqrt{\frac{2\pi k T(m_1+m_2)}{m_1 m_2}}\left(\frac{kT}{\pi\sigma_{12}^2\Omega^{(1,1)}(\Theta)p}\right)$$

The influence of the dipole moment of the gas is treated by the scaling parameter (Brown *et al.* 2011)

$$\xi = 1 + \frac{\bar{\alpha}\bar{\mu}^2}{16\pi\epsilon_0}\sqrt{\frac{\varepsilon_1}{\varepsilon_2}},$$

where the reduced dipole moment is given by

$$\bar{\mu}^2 = \frac{\mu^2}{\varepsilon_1\sigma_1^3}$$

and the reduced polarizability of the bath gas is given by

$$\bar{\alpha} = \frac{\alpha}{\sigma_2^3}.$$

The scaling parameter ξ is used in the following combination rules to calculate the well depth of the effective interaction potential

$$\varepsilon_{12} = \xi^2 \sqrt{\varepsilon_1 \varepsilon_2}$$

and the collision diameter

$$\sigma_{12} = \xi^{-1/6} \frac{\sigma_1 + \sigma_2}{2}.$$

The second order correction (Marrero and Mason 1972) is not considered yet. Therefore, the diffusion coefficient of a polar gas in a non-polar bath gas is equal to the diffusion coefficient of a non-polar gas in a polar bath gas. For diffusion of a polar gas in a polar bath gas, this formula cannot be used.

`fit_B_data(B_df)`: Determination of Lennard-Jones parameters σ and ε by nonlinear regression from a data frame of second virial coefficient data. The data frame must contain the columns `T` for the temperature and `value` for the viscosity in units `cm3/mol`.

`fit_viscosity_data(viscosity_df)`: Determination of Lennard-Jones parameters σ and ε by nonlinear regression from a data frame of viscosity data. The data frame must contain the columns `T` for the temperature and `value` for the viscosity in units `uPa.s`.

`fit_B_viscosity_data(B_df, viscosity_df, log=FALSE)`: Determination of Lennard-Jones parameters σ and ε by simultaneous nonlinear regression from a data frame of viscosity data and a data frame of second virial coefficient data using optim.

If `log=FALSE` the function to be minimized is given by (Bechtel *et. al.* 2020)

$$\chi^2(\sigma, \varepsilon) = \sum \left(\frac{\eta(\sigma, \varepsilon, T) - \eta_{\text{exp}}}{\Delta \eta_{\text{exp}}} \right)^2 + \sum \left(\frac{B(\sigma, \varepsilon, T) - B_{\text{exp}}}{\Delta B_{\text{exp}}} \right)^2$$

where

$$\Delta \eta_{\text{exp}} = |\max(\eta_{\text{exp}}) - \min(\eta_{\text{exp}})|$$

and

$$\Delta B_{\text{exp}} = |\max(B_{\text{exp}}) - \min(B_{\text{exp}})|$$

If `log=TRUE` the function to be minimized is given by (Zarkova and Hohm 2009)

$$\chi^2(\sigma, \varepsilon) = \sum \left[\ln \left(\frac{\eta_{\text{exp}}}{\eta(\sigma, \varepsilon, T)} \right) \right]^2 + \sum \left[\ln \left(\frac{|B_{\text{exp}}|}{|B(\sigma, \varepsilon, T)|} \right) \right]^2$$

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Examples

```
## Not run:
# Second virial coefficient of methane at 300 K and standard pressure
CH4 <- Gas("methane")
print(CH4$B(T=300))
# Self-diffusion coefficient at 300 K
print(CH4$diffusion(T=300))
# create an instance of Gas for a molecule not listed in data_frame gas
Hg <- Gas("mercury")
# relative molecular mass
Hg$M <- 200.59
# mass of 1 molecule in kg
Hg$m <- Hg$M / pkg.env$Na / 1000
Hg$sigma <- 2.969
Hg$epsk <- 750
print(Hg$thermal_conductivity(T=700))

## End(Not run)
```

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