NAME

goma — GO MAterials database

SYNOPSIS

goma [**-all**, **-a**] [**-composition** *composition*, **-c** *composition*] [**-density**, **-d**]
[**-dynamic_viscosity**, **-y**] [**-expansion_coefficient**, **-e**]
[**-file** *db.yml*, **-f** *db.yml*] [**-help**, **-h**] [**-heat_capacity**, **-j**]
[**-list** *all|substances|properties*, **-L** *A|S|P*] [**-molar_mass**, **-M**]
[**-quiet**, **-q**] [**-resistivity**, **-r**] [**-sound_velocity**, **-s**]
[**-substance** *symbol*, **-S** *symbol*] [**-surface_tension**, **-u**] [**-Tb**, **-b**]
[**-temperature** *temperature in K*, **-T** *temperature in K*]
[**-thermal_conductivity**, **-t**] [**-Tm**, **-m**] [**-vapour_pressure**, **-p**]
[**-verbose**, **-v**] [**-version**, **-V**]

DESCRIPTION

goma (GO MAterials database) is a program enabling command line access to the YAML materials database files distributed with yamdb. It implements the equations necessary to calculate the thermophysical properties from the coefficients stored in the YAML database.

The options are as follows (long option followed by corresponding short option separated by comma):

-all, **-a**
: calculate all properties available for the substance

-composition *composition*, **-c** *composition*
: composition of mixture in mol%, if "list": show available compositions

-density, **-d**
: calculate the density

-dynamic_viscosity, **-y**
: calculate the dynamic viscosity

-expansion_coefficient, **-e**
: calculate the expansion coefficient

-file *db.yml*, **-f** *db.yml*
: specify the database file

-heat_capacity, **-j**
: calculate the heat capacity

-help, **-h**
: show the online help

-list *all|substances|properties*, **-L** *A|S|P*
: list (partial) content of the database file and exit

all|A all substances, available properties, compositions, and corresponding sources

substances|S
: all substances

properties|P
: all properties for a substance (needs to be specified on the command line, e.g., -S Na)

-molar_mass, **-M**
: show the molar mass of the selected substance

−quiet, **−q**
reduce verbosity (might facilitate automatic parsing of the output)

−resistivity, **−r**
calculate electrical resistivity

−sound_velocity, **−s**
calculate sound velocity

−substance *symbol for substance*, **−S** *symbol for substance*
specify the substance/material by symbol (e.g., "Na", "NaCl", or "CaCl2-NaCl")

−surface_tension, **−u**
calculate surface tension

−Tb, **−b**
show boiling temperature

−temperature *temperature in K*, **−T** *temperature in K*
specify the temperature in K

−thermal_conductivity, **−t**
calculate thermal conductivity

−Tm, **−m**
show melting temperature

−vapour_pressure, **−p**
calculate vapour pressure

−verbose, **−v**
verbose mode

−version, **−V**
output version information and exit

EXAMPLES

List all substances available in the database "/home/user/materials.yml":

```
goma -L S -f /home/user/materials.yaml
```

List all properties that are available for Na in the embedded databases:

```
goma -list properties -substance Na
```

Show the melting and the boiling temperature as well as the molecular mass of uranium:

```
goma -Tm -Tb -M -S U
```

Calculate the density of bismuth at 600 K:

```
goma -T 600 -S Bi -d
```

Calculate all available properties for potassium at its melting temperature (default temperature):

```
goma -S K -all
```

List all compositions available for the mixture CaCl2-NaCl in the database "/home/user/salts.yml":

```
goma -S CaCl2-NaCl -f /home/user/salts.yml -c list
```

Calculate all available properties for CaCl2-NaCl 15-85 at 1100 K:

```
goma -S CaCl2-NaCl -c 15-85 -T 1100 -a
```

SEE ALSO

T. Weier, W. Nash, P. Personnettaz, N. Weber (2023) Yamdb: easily accessible thermophysical properties of liquid metals and molten salts. To be submitted to the Journal of Open Research Software.

G. J. Janz (1992) Data from: NIST Properties of Molten Salts Database (formerly SRD 27), National Institute of Standards and Technology, https://doi.org/10.18434/mds2-2298

https://learnxinyminutes.com/docs/yaml/

https://yaml.org/spec/1.2/spec.html

AUTHORS

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BUGS

This is an ALPHA version. Error handling is sloppy to non-existing. Other bugs are likely to appear. If you encounter one, please inform the author.