

Package ‘AmmoniaConcentration’

December 5, 2016

Version 0.1

Author Monica Serra <monicaserra.bio04@gmail.com> and Felipe Tumenas Marques <tumenas@gmail.com>

Maintainer Felipe Tumenas Marques <tumenas@gmail.com>

Title Un-Ionized Ammonia Concentration

Description Provides a function to calculate the concentration of un-ionized ammonia in the total ammonia in aqueous solution using the pH and temperature values.

License MIT + file LICENSE

URL <https://github.com/tumenas/ammonia>

NeedsCompilation no

Repository CRAN

Date/Publication 2016-12-05 08:27:18

R topics documented:

ammonia 1

Index 3

| | |
|---------|---|
| ammonia | <i>Calculation of un-ionized ammonia (NH₃) in total ammonia aqueous solution</i> |
|---------|---|

Description

The total ammonia in aqueous solution is present in two chemical species: un-ionized ammonia, NH₃, and the ionized form, NH₄⁺. The NH₃ species is the one more toxic for aquatic organisms, but current analytical methods do not permit measurement of NH₃, and NH₄⁺ separately. The concentration of each chemical species in the total ammonia is dependent of a number of factors, with the pH and the temperature being the most important.

The equation presented by Emerson et al. (1975) permits the calculation of the NH₃ fraction from the total ammonia measured in freshwater, as long as you also have the pH and temperature data

from the sample. The calculus first calculates the pK a, which is the ionization constant of the ammonium ion. To calculate the pK a value of the sample, we use the equation:

$$pKa = 0.09018 + 2727.92/T$$

where T is the temperature in Kelvin.

To calculate the fraction of NH₃ , we use the equation:

$$f = 1/(10^{(pKa - pH)} + 1)$$

Note: the equation for pK a is invalid outside the temperature range of 0-50 C (273-323 Kelvin), because is the range where the pK a values used to make the equation were obtained empirically.

Usage

```
ammonia(total_ammonia, temperature, ph, type_of_temperature)
```

Arguments

| | |
|---------------------|--|
| total_ammonia | Total ammonia (NH ₃ + NH ₄) in the aqueous solution |
| temperature | Temperature of the aqueous solution |
| ph | pH of the aqueous solution |
| type_of_temperature | Unit of measure of temperature, "K" for Kelvin, "C" for Celsius and "F" for Fahrenheit |

Value

The function returns a list with all steps of the calculation. pka: the immunization constant; pka_ph: the difference between pka and the informed pH; ten_pka_ph: 10 to the power of pka_ph; nh3: the fraction of NH₃; nh3_mgL: the concentration of un-ionized ammonia in the aqueous solution.

References

EMERSON, K.; RUSSO, R.C.; LUND, R.E. et al. *Aqueous ammonia equilibrium calculations: Effect of pH and temperature*. Journal of Fisheries Research Board of Canada, v.32, p.2379-2383, 1975.

Examples

```
ammonia(5.14, 294.4, 6.9, "K")
ammonia(0.98, 27.7, 8.05, "C")
```

Index

ammonia, 1