Package: AmmoniaConcentration (via r-universe)

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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.

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

NeedsCompilation no

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Repository https://tumenas.r-universe.dev

RemoteUrl https://github.com/cran/AmmoniaConcentration

RemoteRef HEAD

RemoteSha adb88ee514c082662bc872796f8c1d970dc5c734

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Description

The total ammonia in aqueous solution is present in two chemical species: un-ionized ammonia, NH 3 , and the ionized form, NH 4 +. The NH 3 species is the one more toxic for aquatic organisms, but current analytical methods do not permit measurement of NH 3, and NH 4 + 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 NH 3 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 (NH3 + NH4) 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 acqueous 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")
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