

# Package ‘AmmoniaConcentration’

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**Title** Un-Ionized Ammonia Concentration Calculation

**Description** AmmoniaConcentration 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

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ammonia	<i>Calculation of un-ionized ammonia (NH<sub>3</sub>) in total ammonia aqueous solution</i>
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## Description

The total ammonia in aqueous solution is present in two chemical species: un-ionized ammonia, NH<sub>3</sub>, and the ionized form, NH<sub>4</sub><sup>+</sup>. The NH<sub>3</sub> species is the one more toxic for aquatic organisms, but current analytical methods do not permit measurement of NH<sub>3</sub>, and NH<sub>4</sub><sup>+</sup> 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<sub>3</sub> 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<sub>a</sub>, which is the ionization constant of the ammonium ion. To calculate the pK<sub>a</sub> 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 NH<sub>3</sub>, we use the equation:

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

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

### Usage

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

### Arguments

total_ammonia	Total ammonia (NH <sub>3</sub> + NH <sub>4</sub> ) 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 NH<sub>3</sub>; 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")
```

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