

THE TOXICITY OF AMMONIA: A THEORETICAL APPROACH

bttps://doi.org/10.56238/sevened2024.033-005

Antonia Beatriz Cavalcante David Vieira¹

ABSTRACT

Ammonia, a compound of great importance today, is present in agricultural activities and even in the technological industry, such as in the generation of clean energy. This chapter will address a brief analysis of the toxicity of ammonia in the human body through theoretical results using very useful methods of computational chemistry, analyzing the basic and solubility properties of this substance as well as its bioavailability according to the pH change.

Keywords: Ammonia. Toxicity. Bioavailability.

¹ Email: beatrizca3155@gmail.com



INTRODUCTION

Nitrogen existing in nature can be found in the following forms: gaseous nitrogen (N2), nitrite ion (NO2⁻), nitrate ion (NO3⁻), ammonium ion (NH4+) and ammonia (NH3). Ammonia is a gaseous, colorless compound that has a strong unpleasant odor (THANS, 2008).

Ammonia is very present in agriculture as one of the compounds that are excreted after production (SOUSA, *et* al, 2016), as well as in industry as a fuel for the generation of clean energy (YAPICIOGLU; DINCER, 2019).



Three-dimensional structure of ammonia

Source: Antonia Beatriz Cavalcante David Vieira

METHODOLOGY

The three-dimensional structure of ammonia was plotted in the Avogadro program: an open source molecular constructor and visualization tool, in version 1.2.0 (<u>http://avogadro.cc/</u>), indexed to the online server Playground Chemaxon© (https://disco.chemaxon.com/calculators/demo/playground/) for the analysis of microspecies, pKa value and solubility and lipophilicity coefficients.

RESULTS

Ammonia has a molecular mass of 17.03 g/mol and a pKa equal to 8.86, that is, it is a basic compound. This substance coexists with its ionized form (NH4+) and its concentrations can vary according to the pH of the medium (BERNARDI, 2022). At physiological pH (pH = 7.40), the ionized species has a concentration equal to 96.70% and the non-ionized species has a concentration equal to 3.30% (Figure 2).



The partition coefficients (logP) and distribution coefficients (logD) are parameters used as a quantitative measure of the lipophilicity of bioactive compounds (WAGER *et al*, 2016), they are important to understand the behavior of substances in the environment in which they are inserted.

Ammonia has the following values: -0.98 for logP and 0.53 for logD, that is, the value of the partition coefficient indicates that the ammonia has good solubility, and the value of the distribution coefficient, in physiological pH, less than 1, indicates that the compound has a low absorption due to its high permeability, and also have a high renal elimination (KAH; BROWN, 2008).



Source: Antonia Beatriz Cavalcante David Vieira

CONCLUSION

Through the analyses presented, it is understood that ammonia is toxic in the human body and the physiological pH can interfere with the bioavailability of the compound due to its unfavorable oral absorption, however, it is worth mentioning that in controlled quantities, ammonia will be dissolved in the body, will not be absorbed and will have a high tendency to be eliminated renally.



REFERENCES

- 1. Bernardi, F. (2022). Uso de quitina e quitosana como adsorventes de amônia de efluentes aquícolas: Revisão de literatura. *Arquivos de Ciências Veterinárias e Zoologia da Unipar*, *25*(2), 1-14.
- 2. Kah, M., & Brown, C. D. (2008). LogD: Lipophilicity for ionisable compounds. *Chemosphere*, *72*, 1401-1408.
- Sousa, F. C., et al. (2016). Medidas para minimizar a emissão de amônia na produção de frangos de corte: Revisão. *Brazilian Journal of Biosystems Engineering*, *10*(1), 51-61.
- 4. Thans, F. C. (2008). *Controle operacional de reator em bateladas sequenciais (RBS): Ajustes na concentração de oxigênio dissolvido visando a remoção de nutrientes* (Dissertação de Mestrado em Engenharia Ambiental). Universidade Federal de Santa Catarina, Florianópolis.
- 5. Wager, T., et al. (2016). Central Nervous System Multiparameter Optimization Desirability: Application in drug discovery. *ACS Chemical Neuroscience*, *7*(3), 767-775.
- 6. Yapicioğlu, A., & Dincer, I. (2019). A review on clean ammonia as a potential fuel for power generators. *Renewable and Sustainable Energy Reviews*, *103*, 96-108.