

Understanding interactions between amino acids and nontronite clays: What is the effect of ions?

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Amino acids are part of the building blocks of life as we know it. Furthermore, they are not only detected on Earth but throughout the universe. However, when exposed to the extreme environments found in space these potential signs of ancient life can quickly decompose. Despite this, it is known that certain mineral surfaces can adsorb and effectively protect these biomarkers from degrading conditions. Therefore, mineral matrices have become a prime target location in the search for biosignatures on other planets such as Mars. [1]

To better understand the effectiveness of mineral protection, we examine interactions of 21 proteinogenic amino acids with two nontronite clays in the presence of four cations: Na^+ , K^+ , Ca^{2+} and Mg^{2+} . In a large-scale molecular modelling study, we characterise and classify the adsorption mechanisms specific to each combination. We observe that the retention of amino acids is dictated by both clay composition and counterions.

Our results highlight the importance of accounting for the unique ion compositions found in extra-terrestrial environments when predicting the retention of biomarkers. In addition, we demonstrate how molecular simulations can guide the search for biosignatures on Earth and beyond.

[1] McMahon, Bosak, Grotzinger, Milliken, Summons, Daye, Newman, Fraeman, Williford, & Briggs (2018). A Field Guide to Finding Fossils on Mars. *Journal of Geophysical Research: Planets*, 123, 1012–1040.

