

Do Silicate Minerals Stabilize Ribose as well? Miguel Fuentes-Cabrera¹, Judit E. Sponer², Jiri Sponer², Alvaro Vazquez-Mayagoitia³, Scott R. Horton¹, Bobby G. Sumpter¹. ¹Oak Ridge National Laboratory, Center for Nanophase Materials Science, Oak Ridge, TN 37831 USA, fuentescabma@ornl.gov; ²Academy of Sciences of the Czech Republic, Institute of Biophysics, CZ-61265 Brno, Czech Republic, judit@ncbr.chemi.muni.cz; ³University of Tennessee, Department of Chemistry, Knoxville, TN 37996 USA

Introduction: The term “RNA world” stands for the theory that presumes that RNA played a critical role in the origin of life, and it hypothesizes that on Early Earth, RNA functioned as both a carrier of genetic information and an enzyme that catalyzed the synthesis of other RNAs. Although this theory received considerable impetus after catalytic RNAs were discovered, its plausibility still remains controversial. For example, one of the main objections is that D-ribose, a component of RNA, could not have accumulated under pre-biotic conditions.

Ribose and related aldopentoses (arabinose, lyxose and xylose), are formed during the formose reaction [1], but whether this reaction could have led to the accumulation of ribose, is a question of debate [2]: ribose has a very short half-life for decomposition at neutral pH and is unstable at acid and basic conditions; this led Larralde *et al.* [3] to conclude that it is unlikely that the backbone of the first genetic material would have contained ribose. New findings, however, cast a different light on this issue: in Ref. [4], Ricardo *et al.* have found that borate minerals do not interfere with the formose reaction and, more importantly, stabilize ribose. As borate minerals are not excluded from Early Earth, Ricardo *et al.* argued that the accumulation of ribose could not be ruled out either. Subsequently, Li *et al.* [5] found that ribose has the strongest affinity for boron, followed by lyxose, arabinose, and xylose, a result which implies that in the presence of borate minerals nature would have preferred accumulating ribose over the other three aldopentoses.

Recently, we carried out a series of theoretical studies [6] to disclose the factors governing the stability of the 2:1 aldopentose-boron complexes. Using a technique based on Density Functional Theory with inclusion of solvation effects, we have shown that the reason for the higher stability of the 2:1 ribose-boron complex is due to (i) the ribose 3-OH is involved in a H-bond with one of the borate-oxygens and (ii) its 5-CH₂OH group is well separated in space from the negatively charged region of the complex and ensures favorable contact with the aqueous medium.

This presentation contains our results on the stability of the 2:1 aldopentose-boron complexes and those we have obtained recently on the stability of the 2:1 aldopentose-silicon complexes. The motivation for

including silicon in our studies is linked to a very interesting paper by Kirschvink *et al.*

In Ref. [7], Kirschvink *et al.* elaborated on Ricardo's *et al.* findings [4] by questioning whether borate minerals could have existed in Early Earth in concentrations high enough to play a role in life's origin. Kirschvink *et al.* concluded that such concentrations are more likely to have existed in Early Mars than in Early Earth, and suggest that life could have started on Mars and then travelled on meteorites to Earth. This conclusion is very intriguing, not only because the images it conjures but also because it prompts two new questions: which minerals could have existed in Early Earth at the required high concentrations?, and could those minerals have stabilized ribose?

Silicate minerals could be an answer to the first question. As for an answer to the second, the experimental study of Lambert *et al.* [8] provides a stepping stone: when studying the silicate complexes of sugars in aqueous solution, they found that among the four aldopentoses, only ribose was able to form a significant amount of the silicate. This led them to conclude that silicate minerals could have played a role in prebiotic chemistry, and to suggest that this issue should be examined in detail.

We examine here this issue, and we have found that all four 2:1 aldopentose-silicon complexes have similar stabilities. This means the four aldopentoses should compete for binding to Si. Furthermore, when comparing our results for the 2:1 aldopentose-boron complexes with those for the 2:1 aldopentose-silicon complexes, we reach the conclusion that silicate minerals should be less efficient than borate minerals in stabilizing ribose.

So is Kirschvink right? Are we all Martians in origin? Before answering this, it would be wise to carry out experiments to address how silicate minerals might stabilize ribose. These experiments should be similar to those performed in Ref. [4].

References:

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