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Life Origination Hydrate hypothesis (LOH-hypothesis): computer simulation of rearrangement of different DNA components within CH_4-hydrate structure II

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Abstract

Three-dimensional simulation confirms the possibility of DNA housing and formation of DNA double helixes within hydrate structure II and, thus, counts in favor of the LOH-Hypothesis for any planet.

1. Introduction

The Life Origination Hydrate Hypothesis (LOH-hypothesis) is based on the notion of life origination as a result of thermodynamically controlled, natural, and inevitable processes governed by universal physical and chemical laws. Just the origination of nucleic acids in the process of evolution of minerals to living organisms is considered by us as the onset of the simplest precellular life. Once nucleic acids had originated and propagated and a medium appropriate for their existence and replication had appeared, the appearance of cellular life was merely a matter of time. DNA-like molecules could be synthesized by Nature only within a mineral matrix, because no explanations of limitation of sizes of the DNA functional groups, their regularity, and the DNA monochirality are, in our opinion, impossible. According to paleontology and logistic, similar DNAs originated repeatedly and DNA ensembles originated compactly. All DNAs, RNAs, and cells should be produced by Nature from three abundant mineral substances, because the meeting of more than three substances together at one point is of low probability. The most appropriate mineral matrix for living-matter origination is hydrate of methane (or, maybe, of other hydrocarbon). The unique triple of minerals capable of forming any DNA, amino-acids, and cells is as follows: CH_4, NO_3^-, and PO_4^{3-}. In accordance with the aforesaid, the LOH-Hypothesis is based on the statement that living organisms originated within the methane-hydrate structure from methane, and nitrate and phosphate ions. This hypothesis was supported by our experimental and observational data available in [1–3] for free. We showed there and earlier in the two-dimensional coordinate system that the sizes of the DNA components correspond to the sizes of the large and small cavities of CH_4-hydrate structure II. However, two-dimensional consideration gives insufficient knowledge on the possibility of housing DNA components within the three-dimensional hydrate structure. In [1], we noted that a group of tasks can be put for computer simulation of rearrangement of different DNA components within hydrate structure II. At present, we solved a number of these tasks, and this is the first presentation of these solutions. The original simulation programs of the type «structure within structure» and procedures are detailed in [4].

3. Simulation results

As is described in [4], we calculated CH_4-hydrate structure II (Fig. 1) and the structures of cytosine, guanine, and desoxy-guanosine complex and their arrangements within CH_4-hydrate structure II.

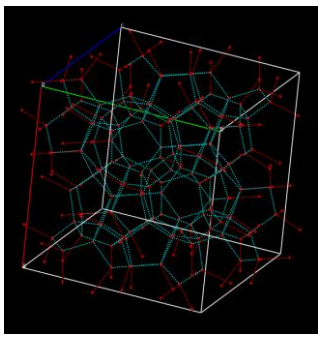


Figure 1: Calculated H_2O structure in CH_4-hydrate II consisting of large ($5^{12}6^4$, d=0.69 nm) and small (5^{12}, d=0.48 nm) cavities. Space group ~Fd3m, a≈b ≈c≈1.685 nm, α≈β≈γ≈90°: red points are O-atoms, green dashes are edges of structural cavities (sum of O–H bond of H_2O and O….H intermolecular bond); red dashes are edges of adjacent cavities; unit cell contains 136 waters.

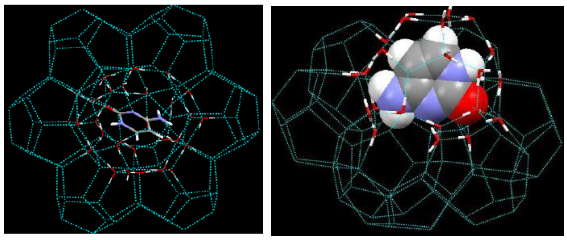


Figure 2: Cytosine (Cy) within a large cavity.

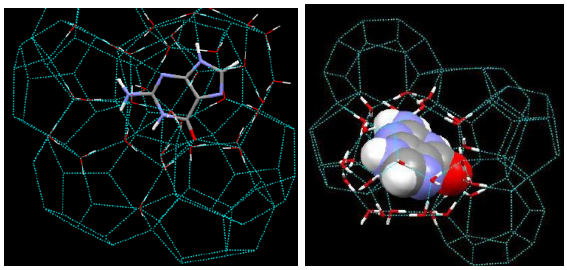
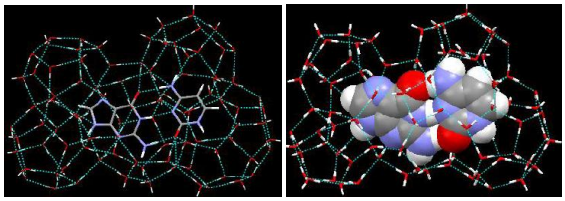
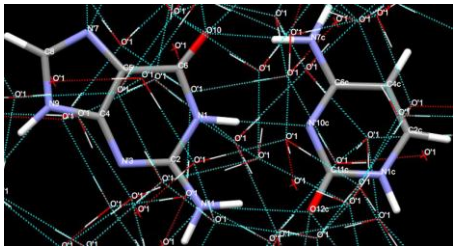


Figure 3: Guanine (G) within a large cavity.



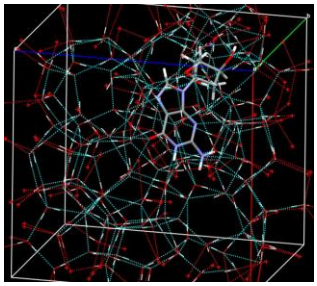
a b



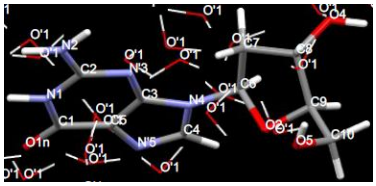
c

Figure 4: H-bound G and Cy within adjacent large cavities: C, O, and N are symbols of atoms; green dashed lines are G…Cy and H_2O…H_2O H-bonds.

The calculations showed the following: (1) nitrogen bases (Figs. 2, 3) and desoxy-ribose (Fig. 5a) can be housed within hydrate cavities and occupy them entirely; (2) calculated H-bonds (Fig. 4c) (nm) O10…N7c (0.287), N1…N'10c (0.295), and N11…O12c (0.288) correspond well to the values [5] 0.293, 0.296, and 0.293, respectively, measured by X-ray method; (3) calculated N4–C6 (Fig. 5b) and measured by X-ray method G–desoxy-ribose chemical bond is equal to (nm) 0.1475 and 0.1509 [6], respectively. Thus, the simulation confirms the compatibility of DNA and hydrate structure II; it also shows that the DNA double helixes can be formed within the hydrate structure.



a



b

Figure 5: (a,b) Desoxy-guanosine complex within hydrate H_2O-network.

Acknowledgements

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References

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