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Life Origination Hydrate Theory (LOH-Theory) and Mitosis and Replication Hydrate Theory (MRH-Theory): three-dimensional PC validation

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Abstract

Size compatibility of the CH_4-hydrate structure II and multi-component DNA fragments is confirmed by three-dimensional simulation; it is validation of the Life Origination Hydrate Theory (LOH-Theory).

1. Introduction

According to the Life Origination Hydrate Theory (LOH-Theory) and Mitosis and Replication Hydrate Theory (MRH-Theory), living matter origination and development are governed by the processes of gas-hydrate structure formation/destruction [1–5]; the DNA components and DNAs as whole were first formed within the CH_4-hydrate structure II (CH_4-HS) from CH_4 and NO_3^- and PO_4^{3-} ions, which diffused into the CH_4-HS from outside. The size correspondence of the CH_4-HS large cavities to N-bases and of the CH_4-HS small cavities to riboses and phosphate-ions was earlier proved by two-dimension consideration. Here, it is confirmed by three-dimensional (3D) simulation. This work allows comparison between the lengths of the intra-DNA inter-component bonds measured earlier for crystals [6-11] with those obtained by our PC simulation.

2. Simulation results

We simulated two molecular complexes, four-radical desoxycytidine – 3,5'– bis (dimethyl phosphate) (Cy-DDR-$(Ph(CH_3)_2)_2$) (Fig. 1a) and five-radical dinucleotide, deoxyribose – guanine – phosphate – deoxyribose – cytosine (G-DDR1-Ph-DDR2-Cy) (Fig. 1b) and one H-bound guanine-cytosine complex (G-Cy) (Fig. 4a).

Principally, we divided simulated molecules into rigid radical fragments, housed them into the corresponding neighbor CH_4-HS cavities, and rotated and shifted all them in search of the states, at which the inter-radical distances became of such lengths that the inter-radical bonds could arise and the radicals in the formed molecules could remain within the initial CH_4-HS cavities; details are in [4].

The Cy-DDR-$(Ph(CH_3)_2)_2$ complex is housed within one large (Cy) and adjacent three small (DDR and two $Ph(CH_3)_2$) cavities of the CH_4-HS (Figs. 2a, 3a) and the G-DDR1-Ph-DDR2-Cy complex is housed within two large (G and Cy) and adjacent three small (two DDR and Ph) cavities of CH_4-HS (Figs. 2b, 3 b).

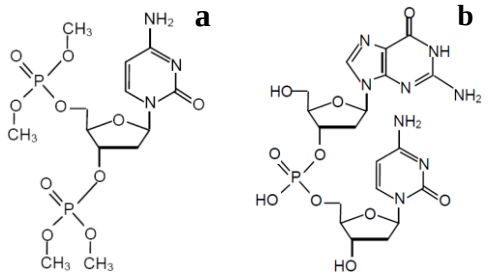

Figure 1: Schemes of the four-radical Cy-DDR-$(Ph(CH_3)_2)_2$ complex (a) and of the five-radical (G-DDR1-Ph-DDR2-Cy) complex (b).

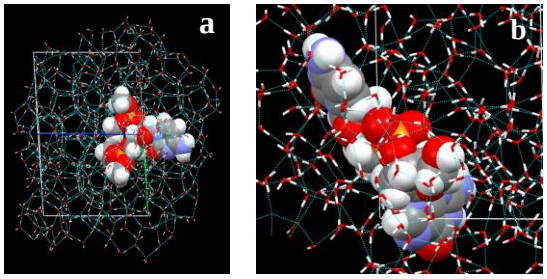

Figure 2: 3D scaled images (Mercury PC program) of the four-radical complex (a) and five-radical complex (b) in CH_4-HS; grey, violet, red, white, and yellow spheres are C, N, O, H, and P atoms, respectively.

The four-radical complex can be housed within the CH_4-HS with no changes in its inter-radical bonds. In the five-radical complex, the N(G)-C(DDR1), C(DDR1)-O(Ph), O(DDR1)-P, P-O(DDR2), O(DDR2)-C(DDR2), and C(DDR2)-N(Cy) bond

lengths (nm) are 1.450 (1.509 [7], 1.47 [8], 1.53 [9]); 1.425 (1.418 [7], 1.43 [8]); 1.568 (1.608 [7], 1.61 [8], 1.56 [9]); 1.570 (1.572 [7], 1.59 [8], 1.56 [9]); 1.413 (1.418 [7], 1.44 [8]); and 1.460 (1.447 [7], 1.47 [8], 1.53 [9]), respectively. In brackets, X-ray data are given. In the G-DDR1-Ph-DDR2-Cy and G-Cy complexes, the simulated and measured bond lengths coincide within experimental errors.

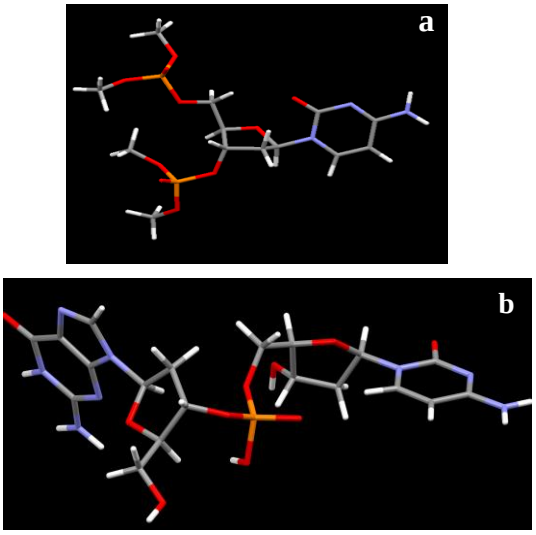

Figure 3: 3D scaled images (Mercury PC program) of the four-radical complex (a) and five-radical complex (b) within the CH_4-HS; grey, violet, red, white, and yellow sticks are the atomic radii of C, N, O, H, and P atoms, respectively, the cross-points of two or more grey, violet, red, and yellow sticks are C, N, O, and P atomic nuclei, respectively, and the points of white stick connections with sticks of any other color are H-atom nuclei. The H_2O structure is removed.

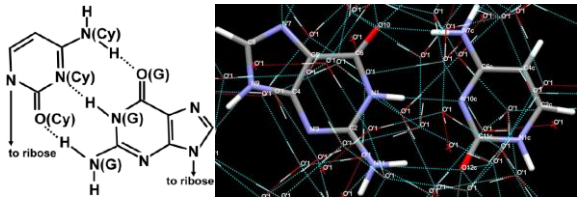

Figure 4: The H-bound G-Cy complex: scheme (a); simulated 3D scaled image within two adjacent large CH_4-HS cavities (Mercury PC program) (b); the N(Cy)…O(G), N(Cy)…N(G), and O(Cy)…N(G) bond lengths (nm) are 2.87 (2.93 [10], 2.84 [11]); 2.95 (2.96 [10], 2.92 [11]); and 2.88 (2.93 [10], 2.84 [11]), respectively. In brackets, X-ray data are given.

3. Conclusion

The data confirm the DNA compatibility with the CH_4-HS and, thus, count in favor of the LOH-Theory.

Acknowledgements

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