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

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I. Introduction: CH_4-hydrate deposites as the cradle of life

DNAs and living cells originated within the solid methane-hydrate matrix deposits in the periods of terminations of the Earth's glaciations.

At present, the major portion of natural gas (methane) is located in many regions of the world ocean at different depths under seabed at around 270 K and under a pressure of gaseous methane.

Methane is there in the form of solid CH_4-hydrate.

At each temperature, CH_4-hydrate and gaseous CH_4 are in equilibrium.

Apparently, in the cold periods of the Earth's glaciations, the upper boundaries of the CH_4-hydrate deposits were closer to the Earth's surface as compared to the present ones.

Gas hydrates are the substances characterized by the occurrence of the H_2O-hydrate structure, the large cavities of which contain molecules or atomic groups of any one composition and small cavities contain molecules or atomic groups of any other composition.

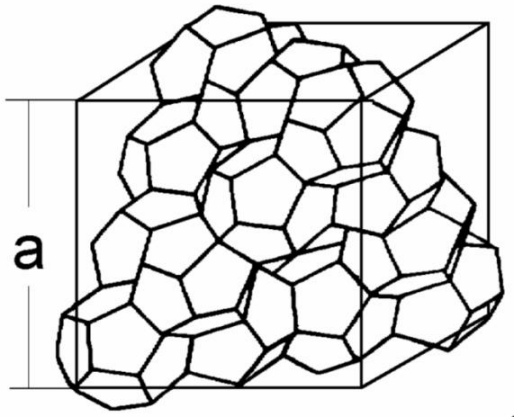
Hundreds of gas-hydrates are known, e.g.,

$C_4H_4O \cdot 17\ H_2O$; $(CH_2)_4O \cdot 17\ H_2O$; $(CH_2)_4O \cdot 2\ H_2S \cdot 17\ H_2O$.

The lattice can be of different modifications, which are capable of transforming to each other;

we consider the so-called structure II.

The CH_4-hydrate crystal lattice has a honeycomb cubic structure.



Methane-hydrate structure II:

Space group ~Fd3m,

$a \approx b \approx c \approx 1.685$ nm, $\alpha \approx \beta \approx \gamma \approx 90^o$.

Each crystal unit cell contains 16 small cavities and 8 large cavities.

The crystal lattice is built of the H-bound H_2O molecules.

Each small cavity is bounded by

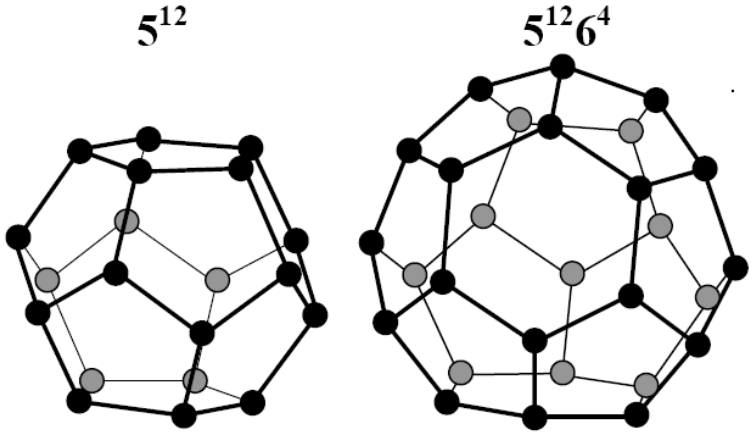
12 regular pentagons and

have a free volume of 4.8 Å in diameter;

each large cavity is bounded by

12 regular pentagons and 4 regular hexagons and

have a free volume of 6.9 Å in diameter



Each O-atom is located at a lattice point.

Each edge connects two neighboring

H_2O molecules and

represents the sum of

intra-molecular chemical O-H bond and

inter-molecular hydrogen O····H bond.

According to our Life Origination Hydrate Theory (LOH-Theory),

the nucleosides formed

within pairs of neighboring large and small CH_4-hydrate cavities

by the reaction

NO_3^- + CH_4

and then PO_4^{3-} ions joined the nucleosides to each other

with formation of DNA-like molecules.

In order that it could occur,

the sizes of large hydrate cavities

should be equal to the sizes of N-bases and

the sizes of small cavities

should be equal to the sizes of ribose and phosphodiester radicals.

At the early step of the theory development,

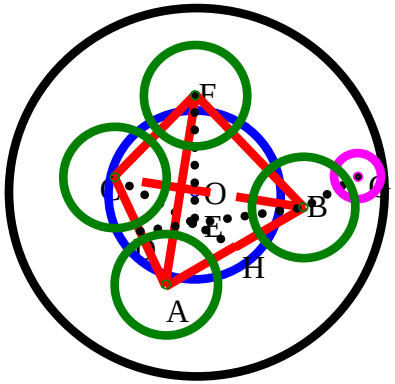
we proved on the basis of two-dimensional consideration

that this condition works (see the next slide).

All the sizes are given here in the same scale.

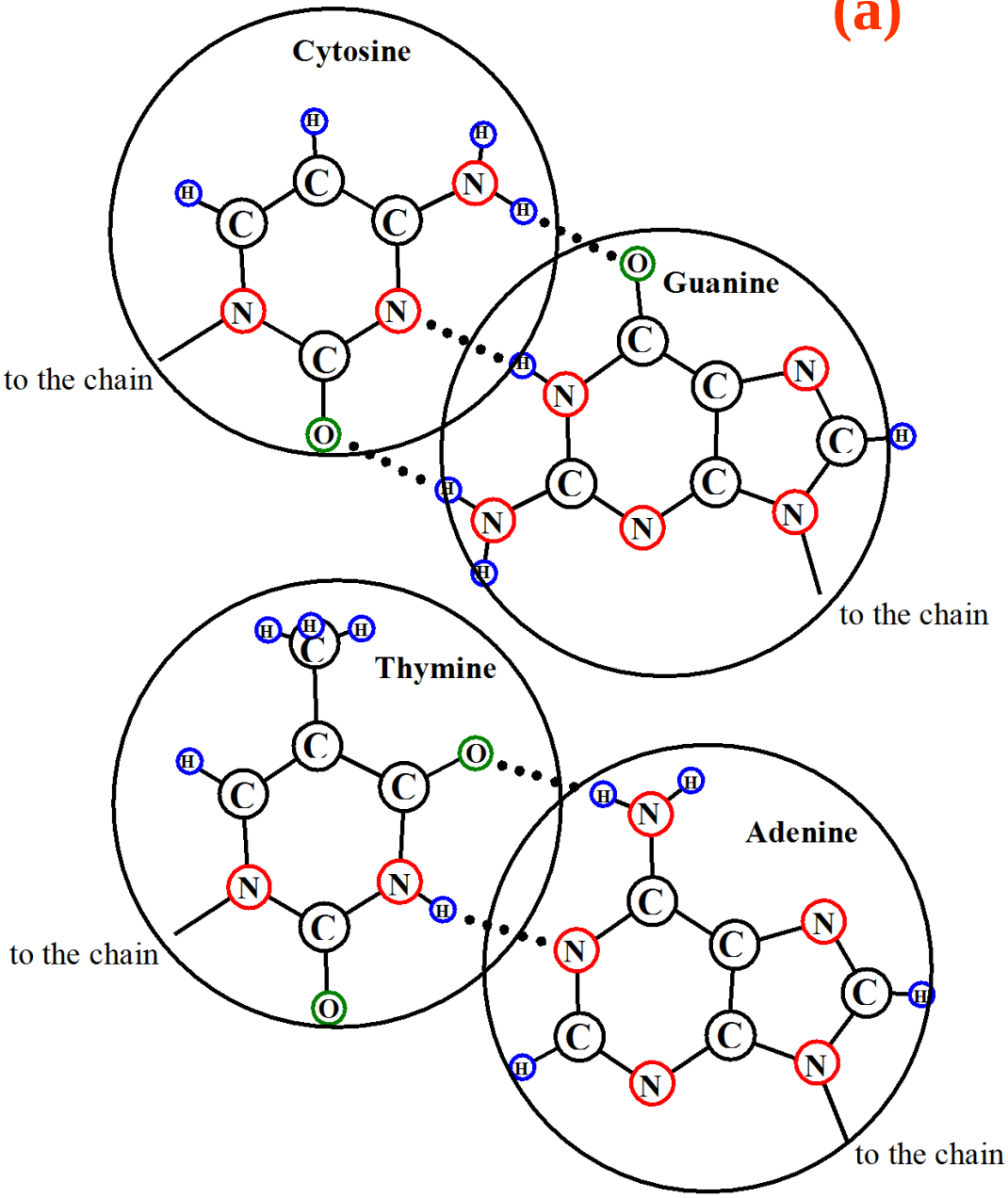
The circles correspond to the sizes of large (a) and small (b) hydrate cavities.

(b)



The large cavities are as if "moulds" for N-bases; the small cavities are as if "moulds" for phosphate groups and riboses.

(a)



To consider the size-correspondence problem in detail,

we developed

an original three-dimensional PC crystallographic program

of the type "a structure within another structure".

The program allows arrangement of rather big DNA fragments

within the gas-hydrate structure cavities

and verification of the degree of compatibility

between the structures of gas-hydrate and DNA-fragments,

namely,

the program allows comparison between the inter-atomic distances

the simulated DNA fragments

and the corresponding available distances

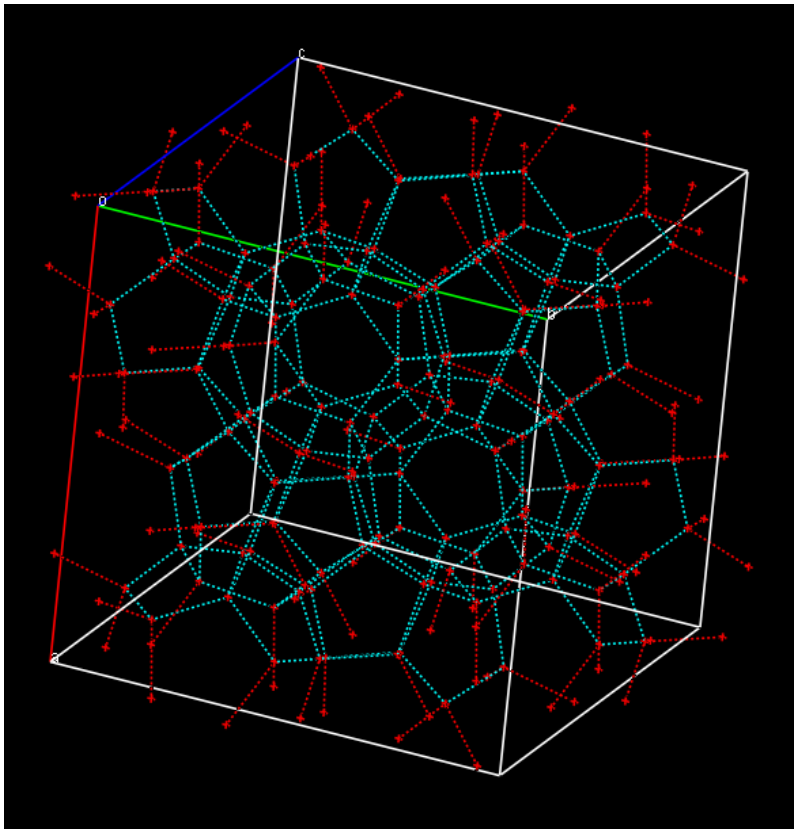
obtained as a result of X-ray studies.

Below, applications of this program to verification of our theory are given.

We consider new results and the results presented at the EPSC2013.

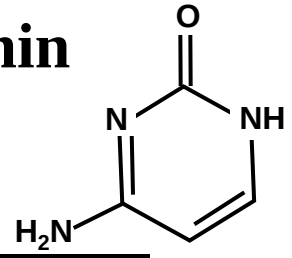
II. Three-dimensional inspection of the correspondence between the sizes of gas-hydrate cavities and DNA components

Calculated unit cell of the gas-hydrate (II) H_2O matrix (the cell contains 136 waters)



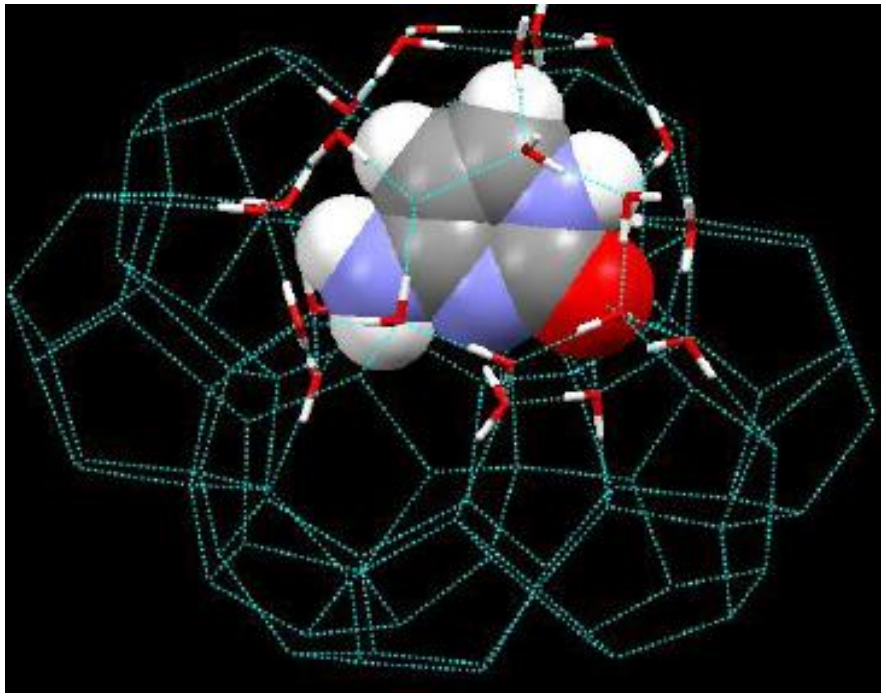
Red points: O-atoms;
green dashes: cavity edges
red dashes: cavity edges beyond the unit cell.

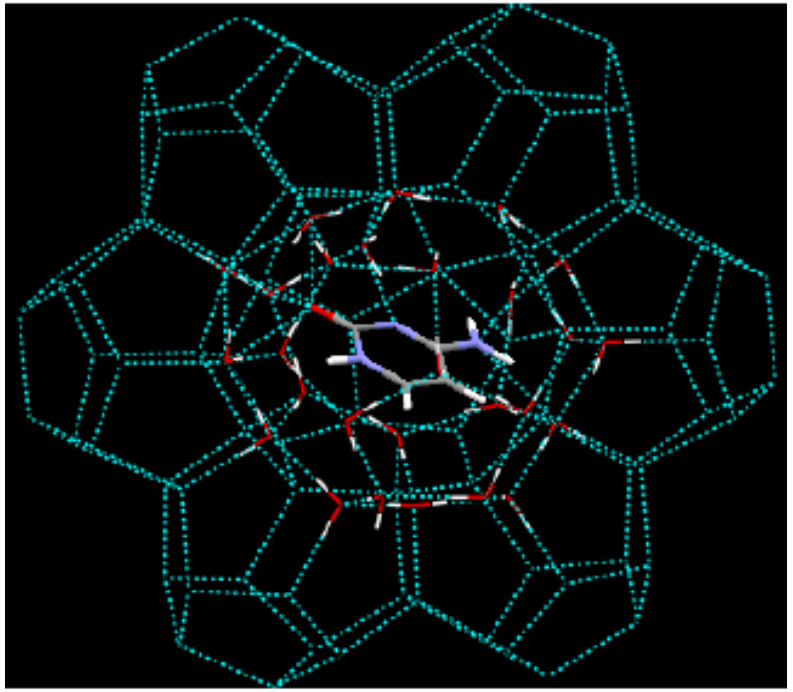
The cytosine (Cy, pyrimidine base) molecule within the large hydrate cavity



Hereafter, the C, N, O, and H atoms are given as the grey, violet, red, and white ones

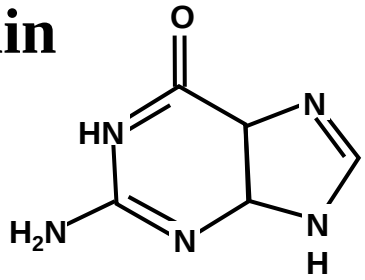
Cy molecules are compatible with CH_4-hydrate large cavities (on the left, 3D image of each atom is given)



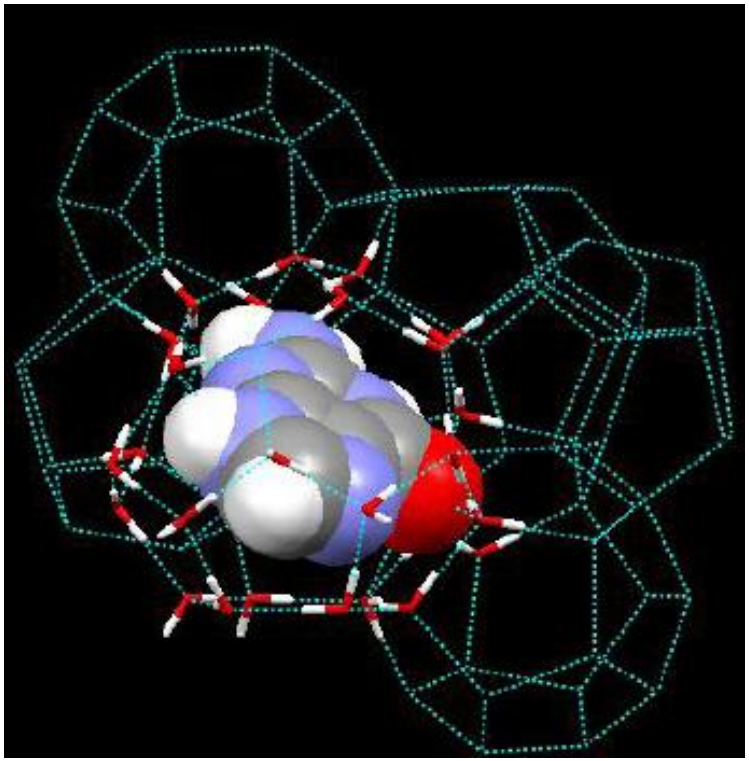


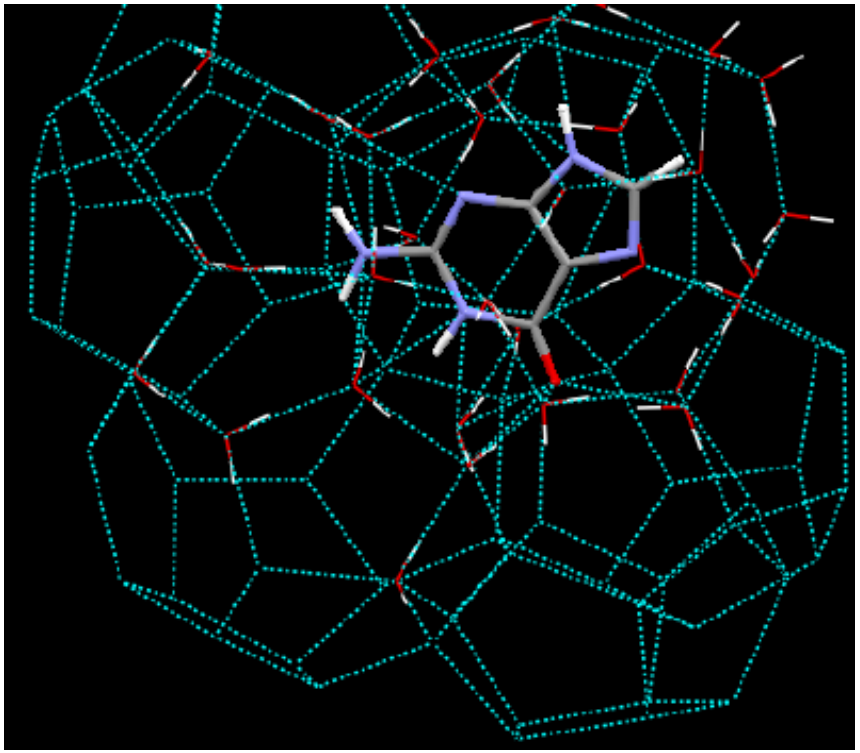
Hydrate structure is conserved, and there is no volume for additional atoms.

The guanine (G, purine base) molecule within the large hydrate cavity



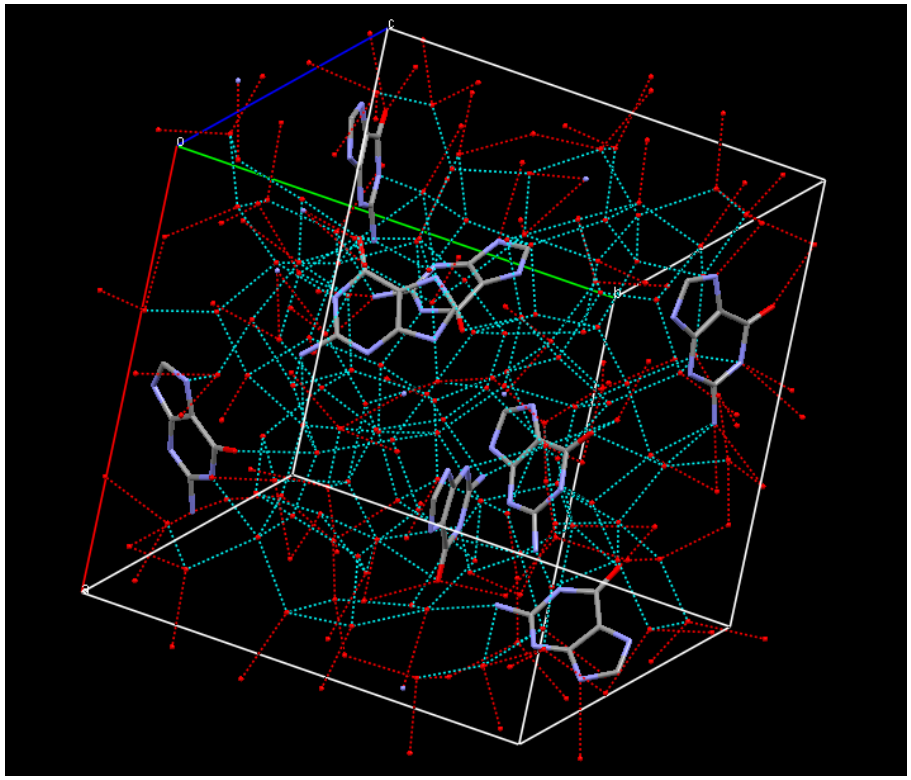
G molecules are compatible with CH_4-hydrate large cavities (on the left, 3D image of each atom is given)

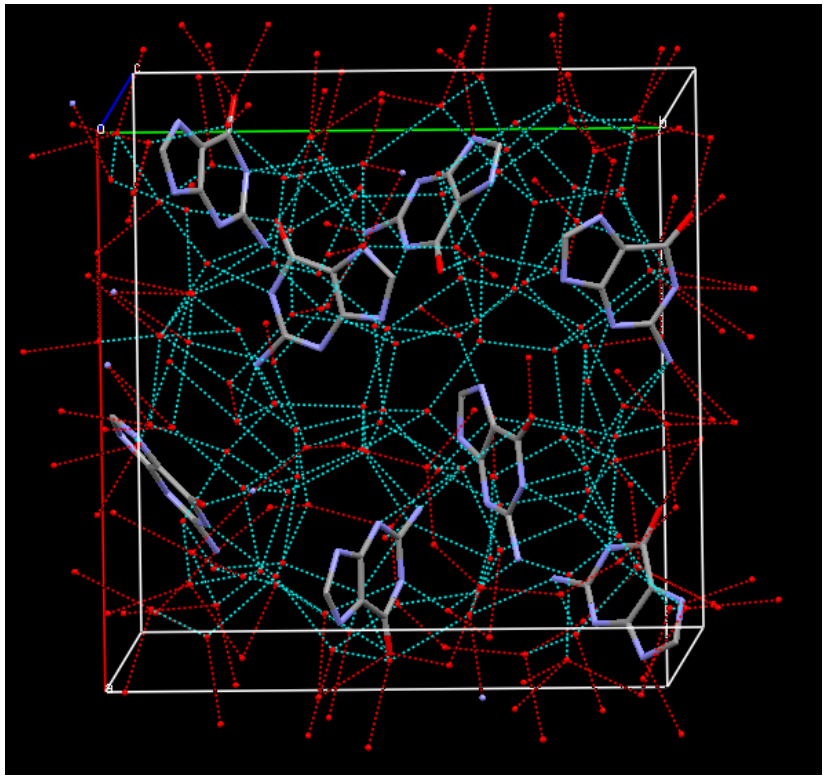




Hydrate structure is conserved, and there is no volume for additional atoms.

May purines be located in close proximity to each other? Here, 8 guanines are housed within 8 large cavities of a unit crystalline cell.



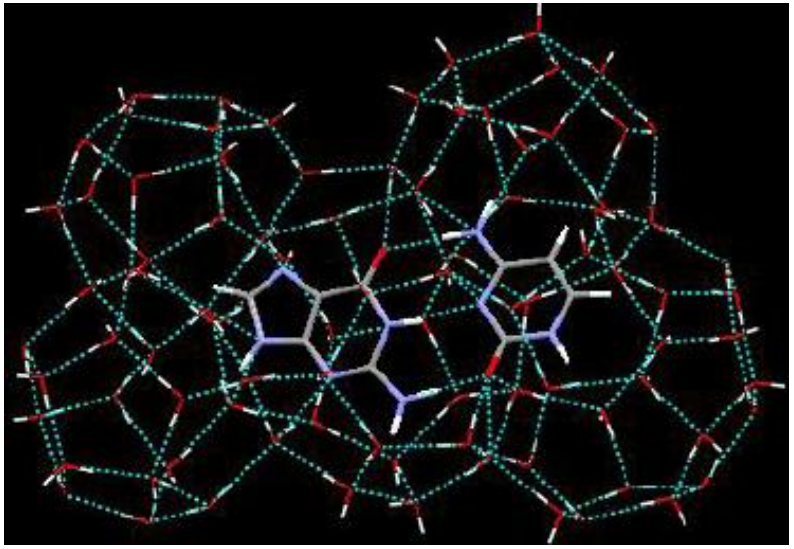


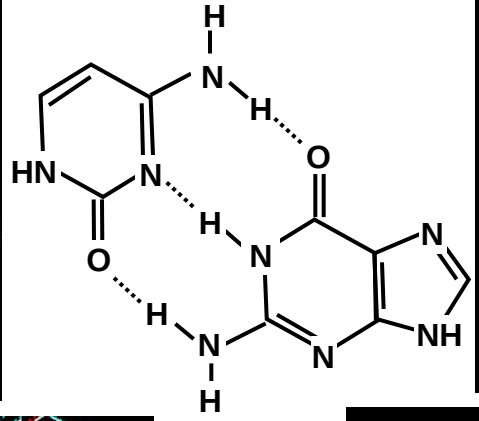
Purines cannot be located in close proximity to each other within the CH_4-hydrate matrix large cavities, because such an arrangement leads to 5% distortion of the matrix.

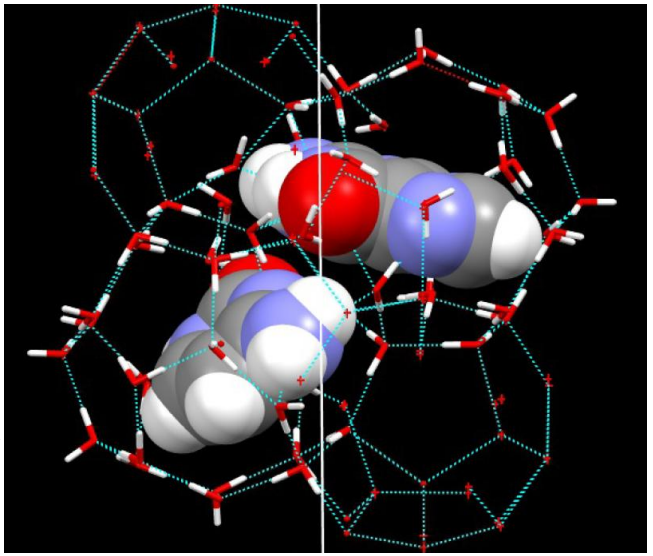
Thus, purines should alternate with pyrimidines.

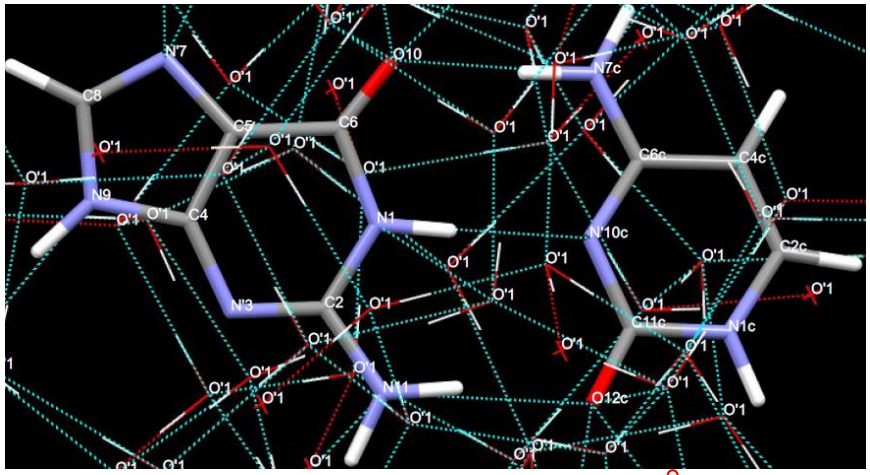
Arrangement of the guanine–cytosine H-bound complex within adjacent large cavities

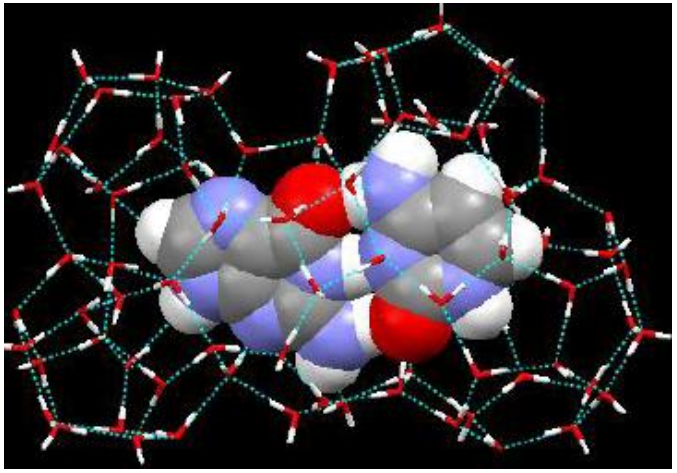
(DNA····DNA H-binding)









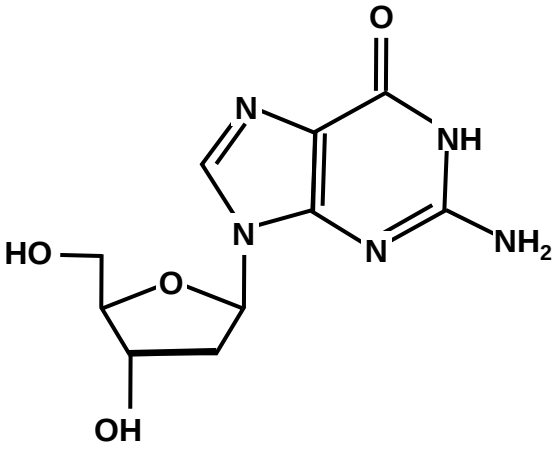


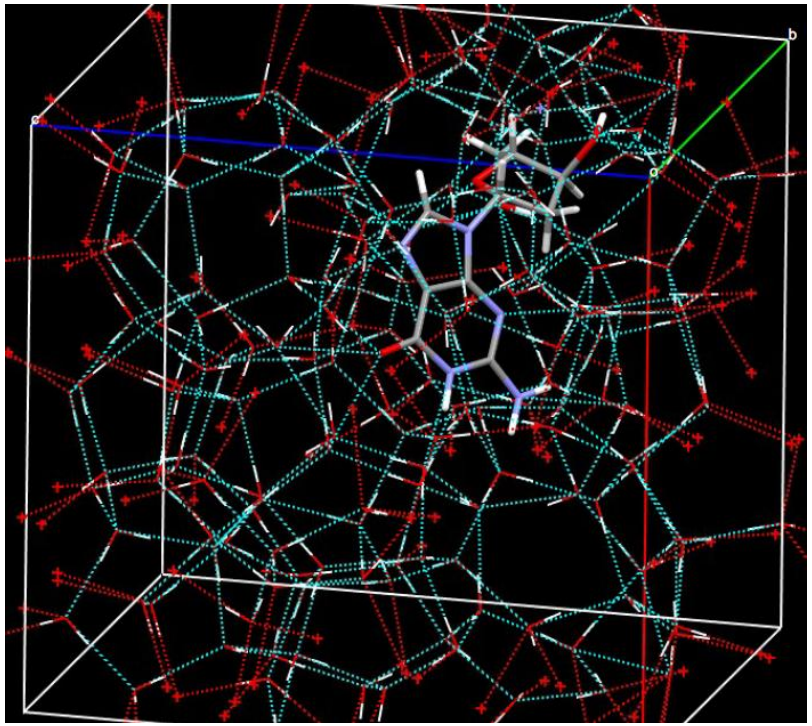
Simulated H-bond lengths (Å): O10···N7c = **2.87**; N11···O12c = **2.88**;

DNA double helix, X-ray data (Å): O10···N7c = **2.93**; N11···O12c = **2.93**.

The possibility of the arrangement is confirmed.

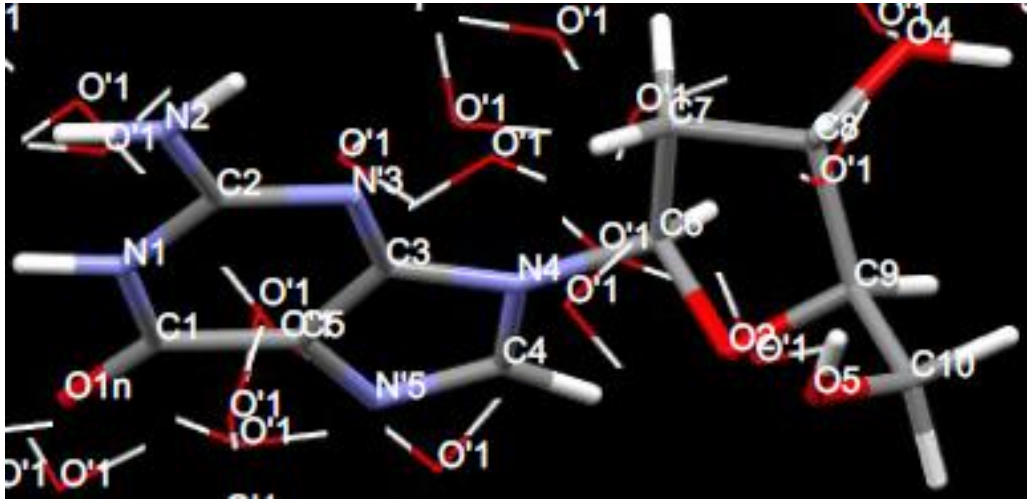
Arrangement of the deoxyribose–guanine complex within adjacent large and small cavities





Simulated N4–C6 bond length (Å): 1.475;

DNA double helix, X-ray data (Å): 1.509

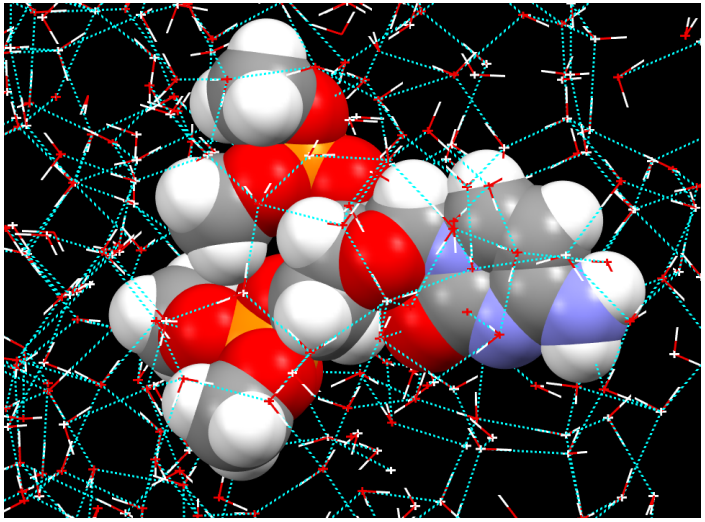


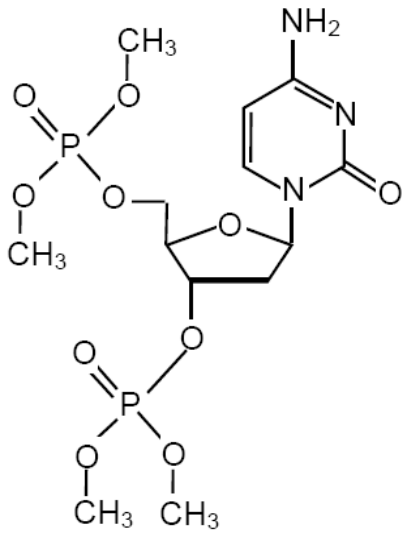
Takusagawa, F., et al., The structure of a pseudo intercalated complex between actinomycin and the DNA binding sequence d(GpC), *Nature* (L), 296 (1982) 466-469.

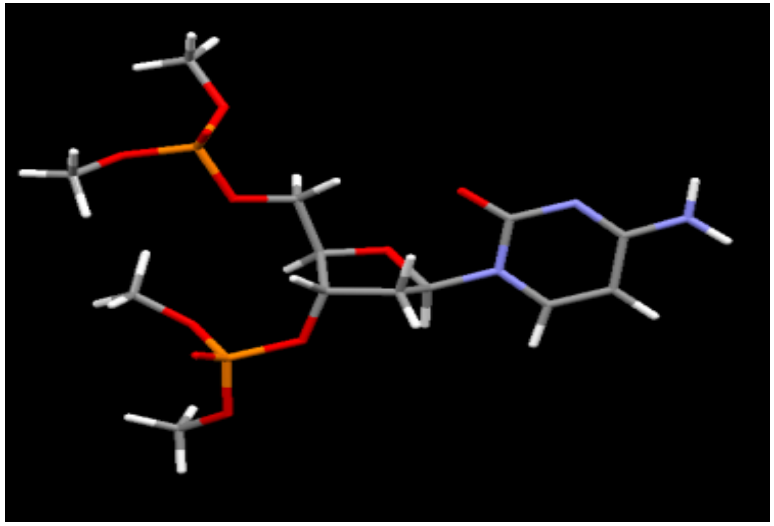
The possibility of the arrangement is confirmed

Arrangement of the 4-radical complex: cytosine/desoxyribose/di-phosphodiester

(in the right figure, the H_2O matrix is removed for clarity)







The bond lengths in the simulated complex are exactly equal to the bond lengths measured by the X-ray technique in crystalline DNA by

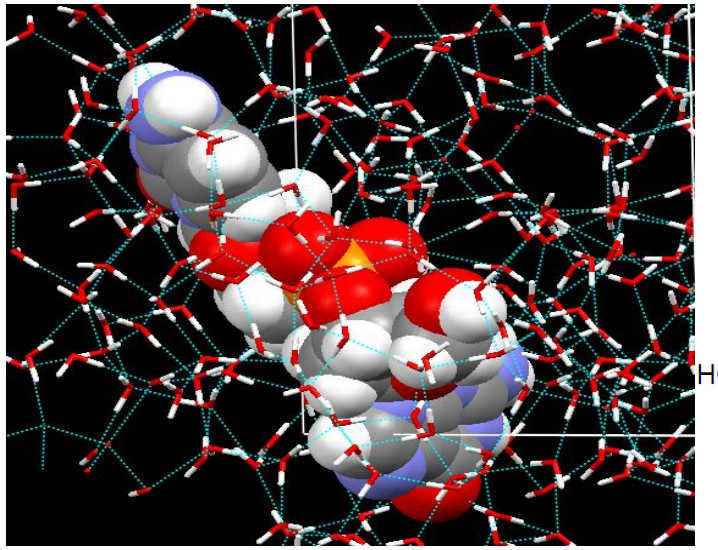
M. Sundaralingam, L. Jensen, J. Mol. Biol., 13 (1965) 914.

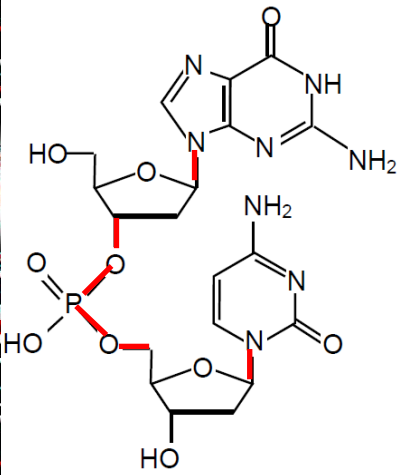
The four-radical complex can be housed within the methane-hydrate matrix with no changes in its inter-radical bonds.

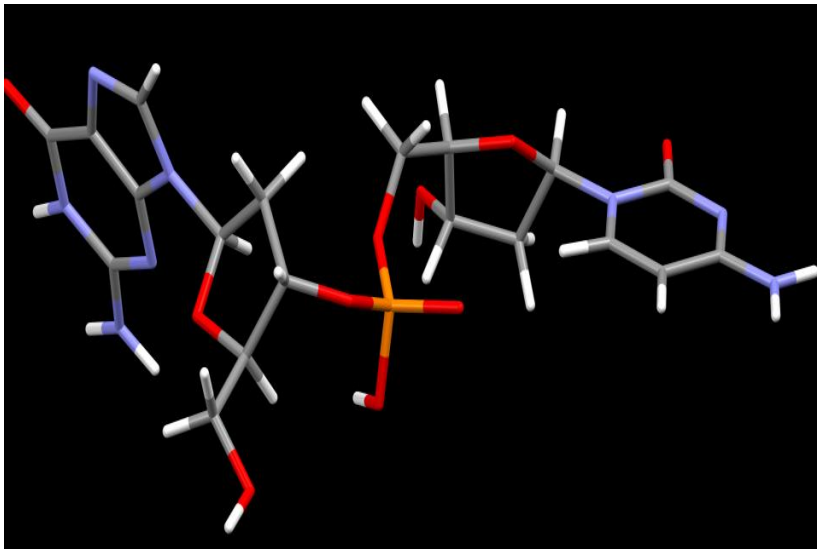
The possibility of the arrangement is confirmed

Arrangement of the 5-radical complex: guanine (G)/desoxyribose (DDR1) /phosphodiester (Ph) /desoxyribose (DDR2)/cytosine (Cy)

(in the right figure, the H_2O matrix is removed for clarity)







Chemical bond	Bond length (Å)			
	Our simulation	X-ray [4]	X-ray [5]	X-ray [6]
N(G) –C(DDR1)	1.450	1.509	1.47	1.53
C(DDR1)–O(Ph)	1.425	1.418	1.43	
O(DDR1)–P	1.568	1.608	1.61	1.56
P–O(DDR2)	1.570	1.572	1.59	1.56
O(DDR2)–C(DDR2)	1.413	1.418	1.44	
C(DDR2)–N(Cy)	1.460	1.447	1.47	1.53

The 5-radical complex can be housed within the methane-hydrate matrix with no changes in its inter-radical bonds (the references are given in Conclusion).

The possibility of the arrangement is confirmed

III. Conclusion

Guanine–cytosine H-bond lengths (Å)

Bonds	O10····N7c	N1····N'10c	N11····O12c
Our simulation	**2.87**	**2.95**	**2.88**
X-ray data [1]	**2.93**	**2.96**	**2.93**
X-ray data [2]	**2.84**	**2.92**	**2.84**

[1] White, A., Handler, P., Smith, E.L., et al.: Principles of Biochemistry, 6th edn., NY, USA, 1978.

[2] Yčas, M.: The Biological Code. Amsterdam: North-Holland Publ. Co., 1969.

Desoxyribose–guanine chemical bond length (Å)

Bond	N4–C6
Our simulation	**1.48**
X-ray data [3]	**1.51**

[3] Takusagama, F., Dabrow, M., Neidle, S., and Berman, H.M.: The structure of a pseudo intercalated complex between actinomycin and the DNA binding sequence d(GpC), Nature (L), 296 (1982) 466–469.

Bond lengths in the five-radical complex: Guanine (G) – Desoxy-D-ribose 1 (DDR1) – Phosphodiester (Ph) – (DDR2) – Cytosine (Cy)

Chemical bond	Bond length (Å)			
	Our work	X-ray [4]	X-ray [5]	X-ray [6]
N(G) –C(DDR1)	1.450	1.509	1.47	1.53
C(DDR1)–O(Ph)	1.425	1.418	1.43	
O(DDR1)–P	1.568	1.608	1.61	1.56
P–O(DDR2)	1.570	1.572	1.59	1.56
O(DDR2)–C(DDR2)	1.413	1.418	1.44	
C(DDR2)–N(Cy)	1.460	1.447	1.47	1.53

[4] Takusagama F. et al., Nature (L), 296 (1982) 466–469.
[2] Nucleic acid database; http://ndbserver.rutgers.edu.
[3] Pauling L. The Nature of the Chemical Bond. Cornell Univ. Press, NY, 1960

Thus, the DNA and methane-hydrate size compatibility is completely confirmed.

These results count in favor of the LOH-Theory.

Acknowledgment

The work is partially supported by

the Russian Foundation for Basic Research,

project nos. 12-05-01082 and 14-03-01091.

Thank you for your interest!