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THEORETICAL CHEMISTRY. -Electronic conduction in DNA and in the DNA-Mg^{2+} complex. Note (*) of Madame Andree Goudot, presented by Prince Louis de Broglie. Compt. Rend. 255:3420-3422, 1962.

Calculation of energy levels of free electrons in the molecules; adenin-thymin, Guanidin-cytosin and adenin-Mg^{2+}-thymin, guanidin-Mg^{2+}-cytosin. The results show debased levels in DNA and DNA-Mg^{2+}. Furthermore there is a conduction band in DNA-Mg^{2+}.

It has been experimentally shown that the conductibility of a solution DNA-Mg^{2+} is greater than that of an aqueous solution of pure DNA (1). On the other hand the electrical properties (2) of DNA have been studied in the form of DNA-Na^{+}.

In the desoxyribonucleic acid the purin-pyrimidin molecules form adenin-thymin and guanidin-cytosin planes which are parallel and which are separated by a distance of only 3.4 Å. There can therefore be interaction between these plane molecules, and in particular a transfer of mobile electrons if molecular energy levels allow it. Whence the interest of this theoretical study of pure DNA and of the complex DNA-Mg^{2+}.

1. DNA. - Calculation of energy levels of mobile electrons and of charges for each of the adenin-thymin and guanidin-cytosin molecules. Those levels are within parallel planes, and may therefore be compared as to their value.

1° Adenin-thymin (AT). - The calculation of the delocalization energy shows that inside the AT molecule a charge neighboring that of two electrons runs from adenin onto thymin. This may be due to two CO groupings, which are strong π "acceptors" of thymin.

2° Guanidin-cytosin (GC) - In the GC molecule guanidin and cytosin each roughly preserve their respective charges.

3° Interactions inside DNA. - a. Occupied levels:

AT : 3.821; 3.690; 3.651; 3.436; 2.467; 2.321; 1.967 and 1.629;

... 3.704; 3.648; 3.590; 3.484; 2.804; 2.527; 2.467; 2.299; 1.759 and 1.322.

The AT and GC molecules have the same energy level (2.467) and this level is a degenerated energy level for the DNA molecule.

c. Lowest free level: for AT : 1.241 and for GC : 1.178.

The lowest free level of AT being situated below that of GC, if an excitation energy permits passage from the highest occupied level (that of GC : 1.322) to the lowest free level (that of AT : 1.241) there will be an electronic transfer from GC onto AT, but this transition cannot continue from AT onto GC, that is along the DNA molecule.

2. DNA-Mg^{2+}. - Mg^{2+} yields octahedric hexavalent complexes. The pyrimidin-Mg^{2+} purin is then a symmetry plane of the complex where Mg^{2+} is connected with four atoms which were connected two-by-two with H connections in pure DNA. Thus, there can be as many metal cations as purin-pyramidin planes in the DNA molecule. The distance between the purin and the pyramidin does not undergo any great variation. In the DNA it is between 2.8 and 3 Å. And since the ion ray of Mg^{2+} is 0.78 Å, we have: Mg^{2+}-O = 1.44 Å and Mg^{2+} - N = 1.48 Å. Whence the distance purin-Mg^2-pyramidin is near 2.92 Å.

1° Adenin-Mg^{2+}-thymin (AT-Mg^{2+}) - As in the case of pure DNA a charge in the neighborhood of two electrons runs from adenin onto thymin.

The highest occupied level for DNA-$^{2+}$Mg (1.632) is very near that of DNA (1.629). But the lowest free level has come near the occupied levels. It is of 1.363 for DNA-Mg^{2+} instead of 1.241 for DNA.

2° Guanidin-Mg^{2+}-cytosin (GC-Mg^{2+}). - Guanidin and cytosin preserve their own charges. The highest occupied level is the same (1.322). The lowest free level and the highest occupied level are getting nearer: 1.285 instead of 1.178.

3° Interactions inside DNA-Mg^{2+}. a. Occupied levels:

AT-Mg^{2+} : 3.843; 3.699; 3.576; 3.479; 2.969; 2.310; 1.966 and 1.632.

GC-Mg^{2+} : 3.797; 3.651; 3.425; 3.307; 2.672; 2.558; 2.467; 2.310; 1.767 and 1.322.

As in pure DNA there is in DNA-Mg^{2+} a debased level (2.310) which is nevertheless situated a little higher.

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b. Lowest free level : for AT-Mg^{2+} : 1.363 and for GC-Mg^{2+} : 1.285.

If we compare the energy levels of free electrons for the purin-pyramidin planes, we have

|	AT-Mg^{2+}		GC-Mg^{2+}
Highest occupied level	1.632	and for	1.332
Lowest free level	1.363		1.285

The lowest free level of AT-Mg^{2+} has a lower energy than the highest occupied level of GC-Mg^{2+}. There may be a spontaneous transition from the highest occupied level of GC-Mg^{2+} on the lowest free level of AT-Mg^{2+} and vice-versa. Those levels are, furthermore, very near each other and form a narrow conduction band. That conduction band makes possible electronic conductibility through DNA-Mg^{2+}. The narrowness of this band makes it very specific. This characteristic makes it possible to explain certain electric properties of those complexes studied in vitro.

Charges. - If we consider charge distribution on each of the plane adenin-thymin- and guanidin-cytosin molecules, since both figures are placed in such a way that a pyrimidin is superposed to a purin and vice versa, we then see that the CO(-0.99) which is most charged with cystin is above the NH$_2$(+0.95) which is most positive of adenin. In return the CO(-0.83) grouping of thymin is situated just above the NH$_2$(+0.36) grouping of guanidin. That may allow Coulomb interactions between those groups (figures 1 and 2).
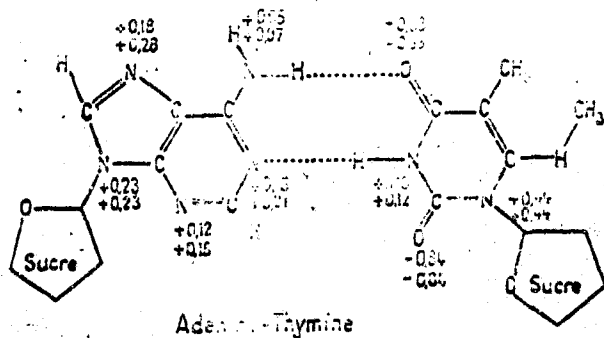
Adenin - Thymine

Fig. 1.
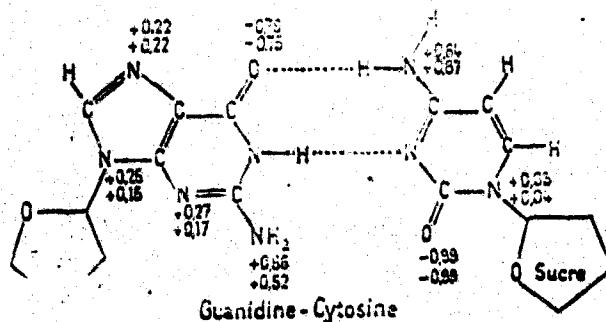
Guanidine - Cytosine

Fig. 2.

Sucre=sugar

3

... show: 1° either that the prop-
... in vivo ... of ... ic compounds of DNA are not to
... vivo ... the DNA; 2° or that in vivo DNA forms an organo
... complex ... but then present the same properties as those found
... those compounds in vitro.

(0) Séance of 5 December 1962.

(1) G. Zubay and D. Doty, Biochem. Biophys. Acta, 1958, p. 51.

(2) P. Denais, C. Sadron and J. Polonsky, Proceedings, 250, 1960, p. 710;
      251, 1960, p. 722.

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