Calculation of the Binding Isotherms of Cu^{2+} and Ca^{2+} Ions Interacting with DNA in Aqueous Solution

Elene V. Hackl **Natalya Bezlepkina** **Yurij P. Blagoi**

hackl@ilt.kharkov.ua

B.I.Verkin Institute for Low Temperature Physics and Engineering,
National Academy of Sciences of Ukraine, 47 Lenin Ave., 310164 Kharkov, Ukraine

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In [1] we have shown that, on its binding to divalent ions studied, DNA transits into the compact state at 29°C and, in so doing, remains in B-form limits. The compactisation process is of positive cooperativity. Model proposed in [1] permits to calculate the binding constants (K_0) of Cu^{2+} and Ca^{2+} ions interacting with DNA on compactisation process as well as the cooperativity parameters (ω) of DNA compactisation process. In the present work we have studied DNA structural transitions under the Cu^{2+} and Ca^{2+} ion action in aqueous solution at higher temperature (45°C) and have calculated the K_0 and ω parameters (see Table 1).

Table 1: Values of binding constants K_0 of divalent metal ions interacting with DNA on compactisation process and cooperativity parameters ω of DNA compactisation process under Cu^{2+} (Ca^{2+}) ions action in aqueous solution at different temperatures.

Metal ion	Temperature, ^{0}C	K_0	ω
Cu^{2+}	29	4.5	9.5
Cu^{2+}	45	10	15
Ca^{2+}	29	0.75	6
Ca^{2+}	45	0.3	5.5

It follows from the Table 1 that with the temperature rise the binding constants K_0 of divalent metal ions interacting with DNA on compactisation process decreases in the case of Ca^{2+}-induced compactisation and increases in the case of Cu^{2+}-induced one. We have shown that in the case of copper ions the determining factor is the increase of binding constants of Cu^{2+} ions interacting with denatured parts formed on DNA while in the case of calcium ions this factor is the decreased screening action of counterions upon the increase of their hydration with temperature. Thus the mechanism of the temperature effect on DNA compactisation in the presence of Cu^{2+} ions possessing higher affinity for DNA bases differs from that of the temperature influence on Ca^{2+}-induced DNA compactisation.

In [1] we also have shown that at ω<8 the binding isotherms (i.e. r dependences on C_f calculated according to formula (2) for the temperature given) are of monotonous character that corresponds to the continuous increase of r with the C_f rise. The isotherm with ω_c =8 having the bending point with the vertical tangent is critical irrespective of the K_0 value. With ω>8 binding isotherms are of S-like form similar to Van-der-Waals ones for liquid-vapour phase transitions. Such binding isotherms have both metastable and absolutely nonstable (with the inverse dependence of r on C_f) parts. In the case of stable complexes such nonmonotonous dependences should be replaced with dependences with a jump along r that is equivalent to the first kind phase transition. As Table shows, the cooperativity parameter of the DNA compactisation process under the action of Cu^{2+} ions at 45°C becomes rather higher than 8, thus, with the temperature increase Cu^{2+}-induced DNA compactisation could gain a phase transition character.

References

[1] Kornilova, S.V., Hackl, E.V., Kapinos, L.E. *et al.*, DNA interaction with biologicaly active metal ions, Cooperativity of metal ion binding at DNA compactization, *Acta Biochim. Polon.*, 45(1):107–117, 1998.