Nuclear Spin Dependent Enzymatic Synthesis of ATP *in vivo* in Strong Magnetic Fields

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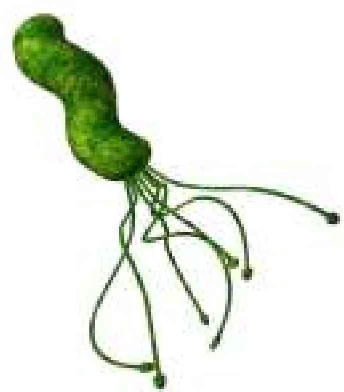
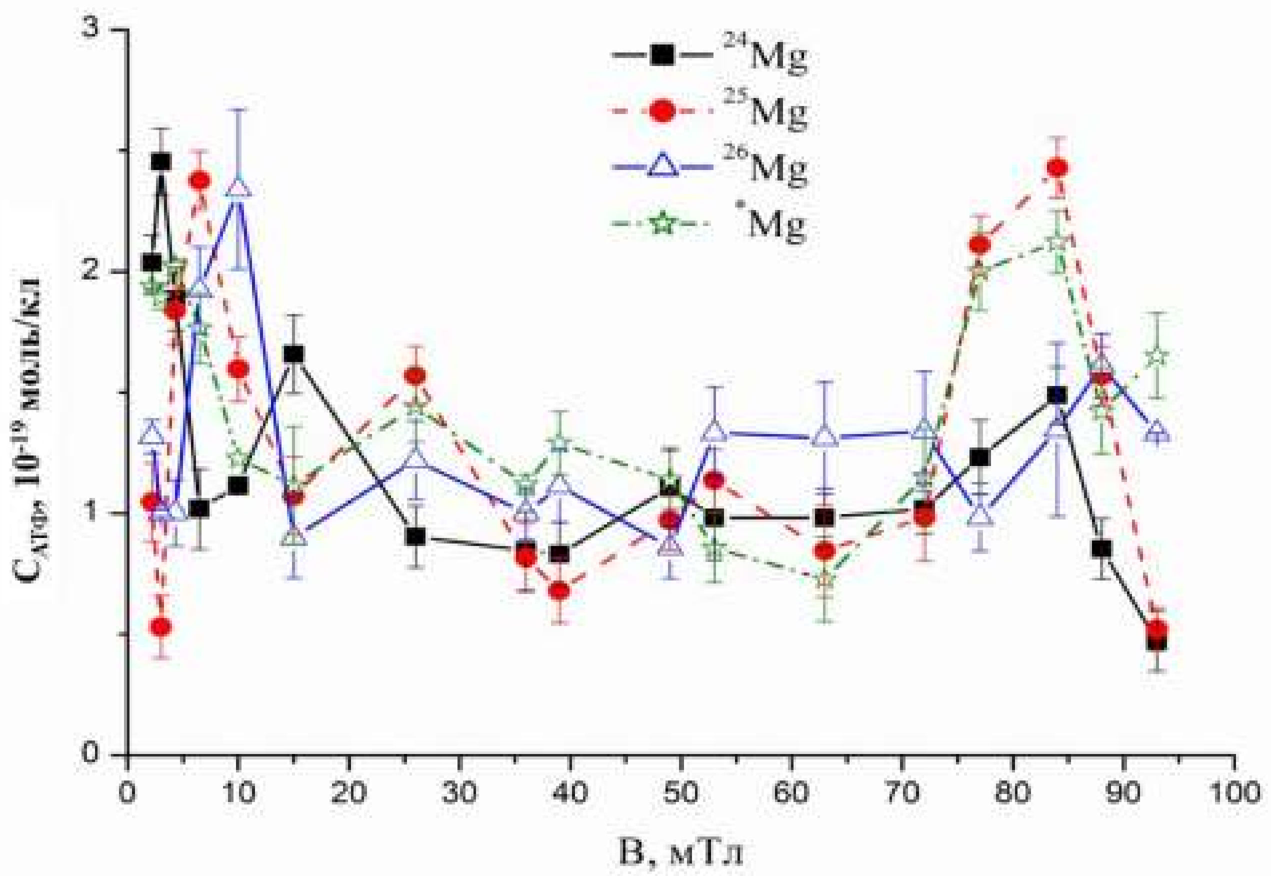
Magnetic field dependence of the ATP pool of *E. coli* bacteria cultured in M9 medium with magnesium isotopes ^{24}Mg, ^{25}Mg, ^{26}Mg, Mg*

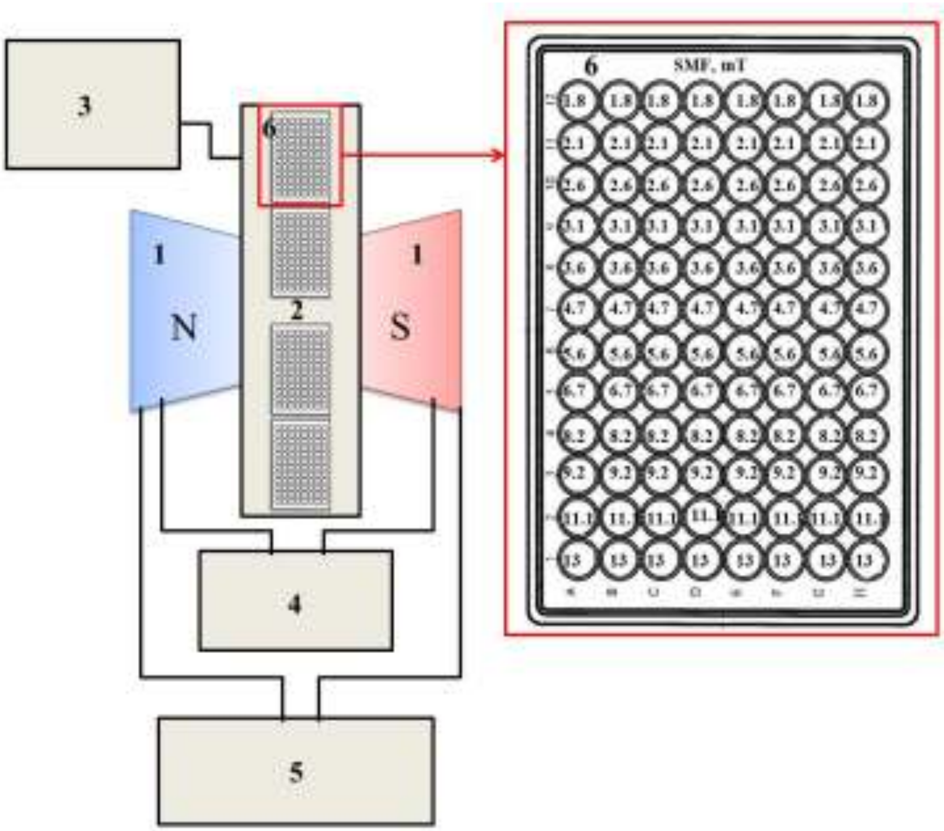
Isotope	Spin
^{24}Mg	0
^{25}Mg	5/2
^{26}Mg	0



Escherichia coli KT12TG1

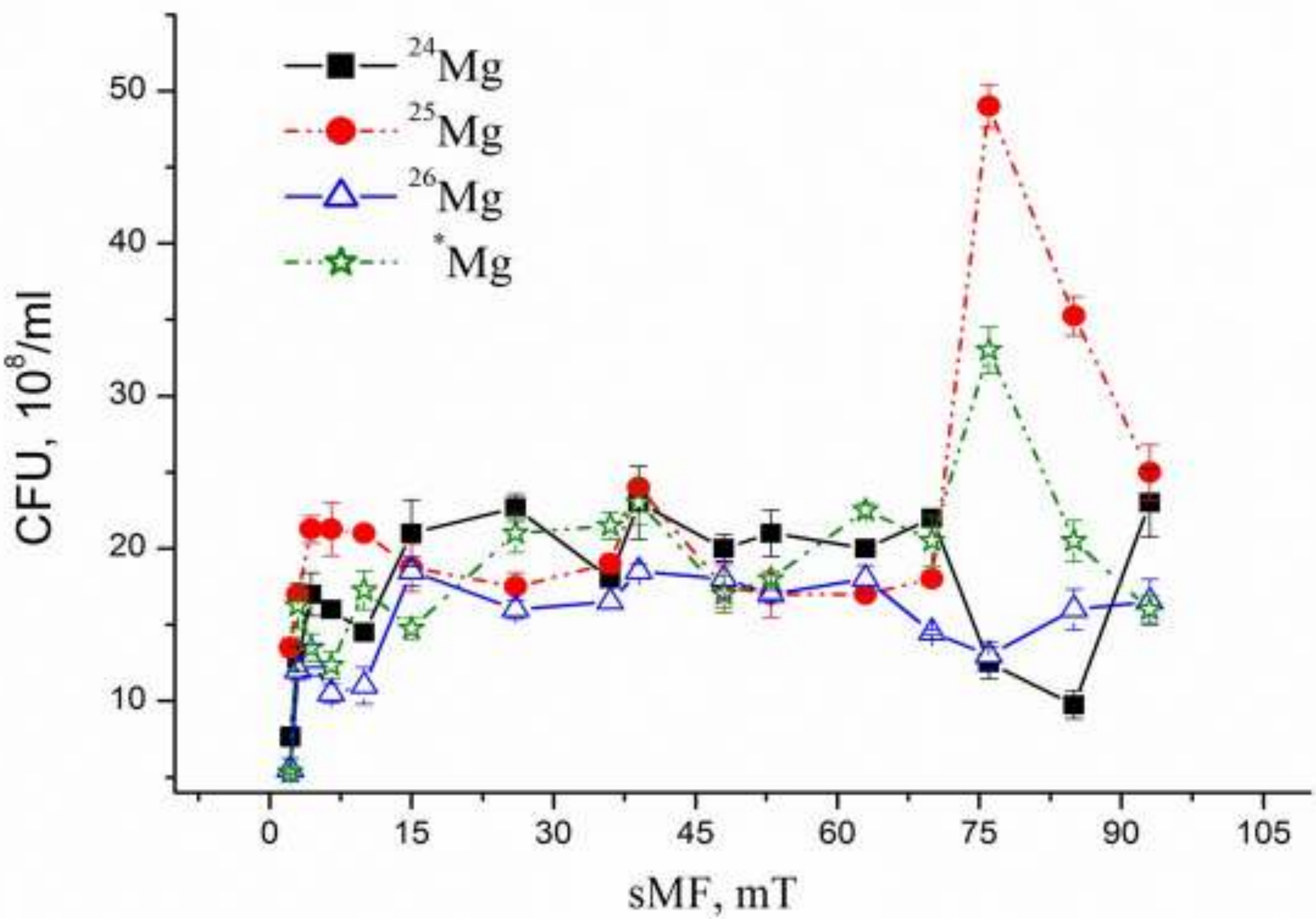


Cultivation of E. coli bacteria on isotopic media in magnetic fields



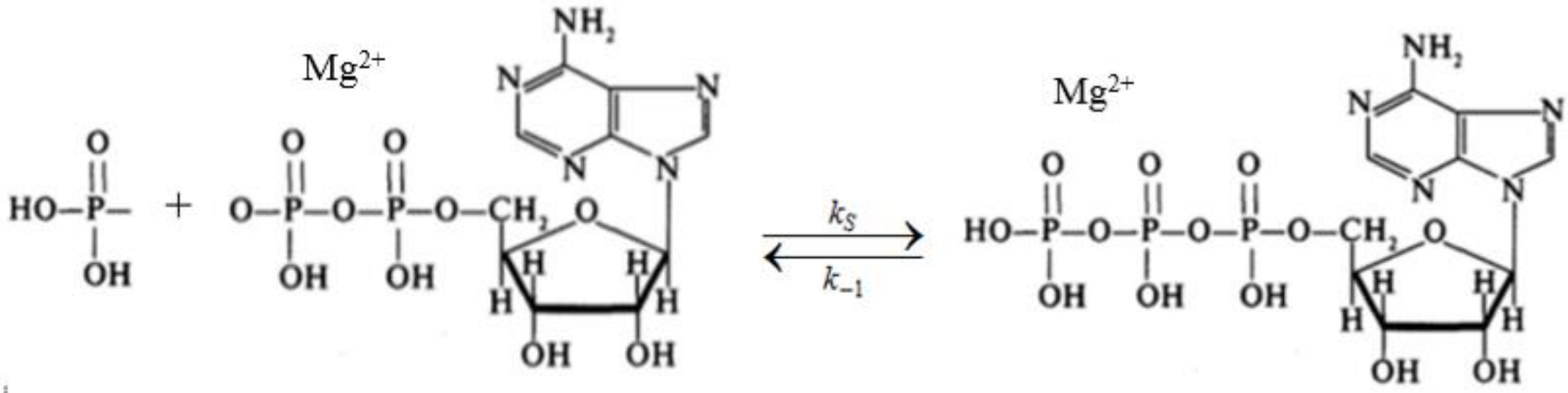
1 – электромагнит;
2 – термостатируемый бокс для культивирования бактерий;
3 – циркуляционный термостат;
4 – блок питания;
5 – система охлаждения;
6 – пример размещения 96-луночной планшеты для культивирования бактерий

Magnetic field dependences of CFU of *E. coli* bacteria cultured on M9 medium with magnesium isotopes



Formal kinetics of intracellular ATP synthesis

Scheme of intracellular synthesis of ATP from ADP and inorganic phosphate PO_3 in the presence of Mg^{2+} ions



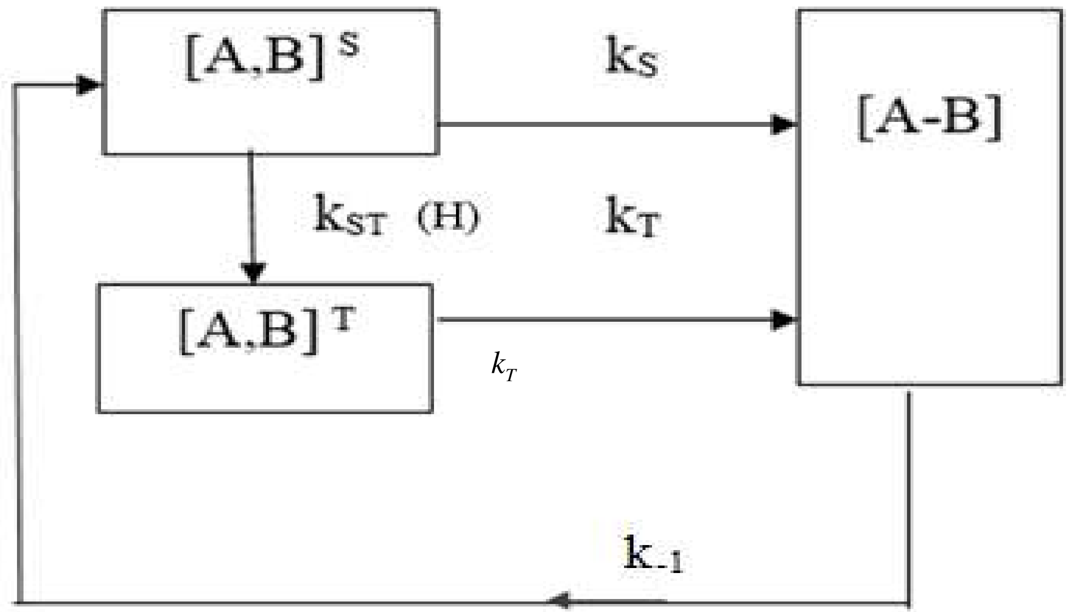
A simple scheme of a reversible reaction

$$\left[A,B\right]\underset{k_{-1}}{\overset{k_S}{\rightleftarrows}}\left[A-B\right]$$

$$[ATP]=[A-B]=\frac{k_S}{k_{-1}+k_S}=\frac{1}{1+(k_{-1}/k_S)}$$

Formal kinetics of intracellular ATP synthesis

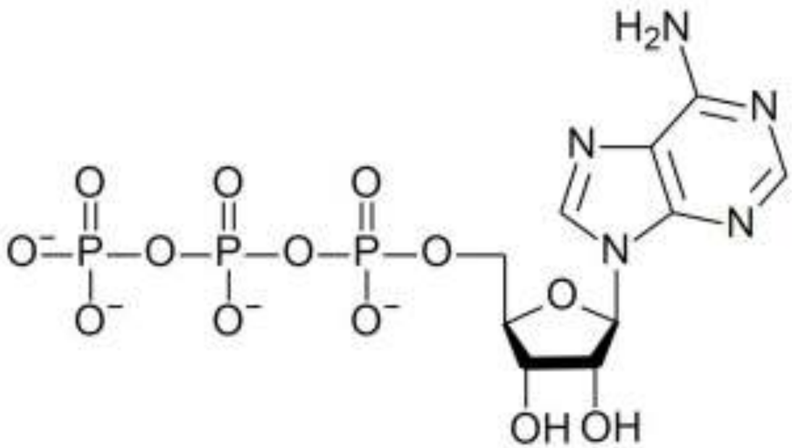
Scheme of the "two-channel" ATP synthesis reaction

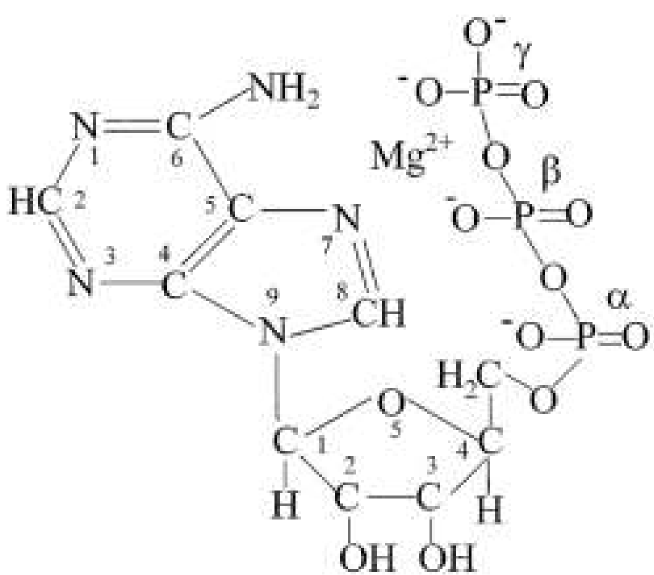


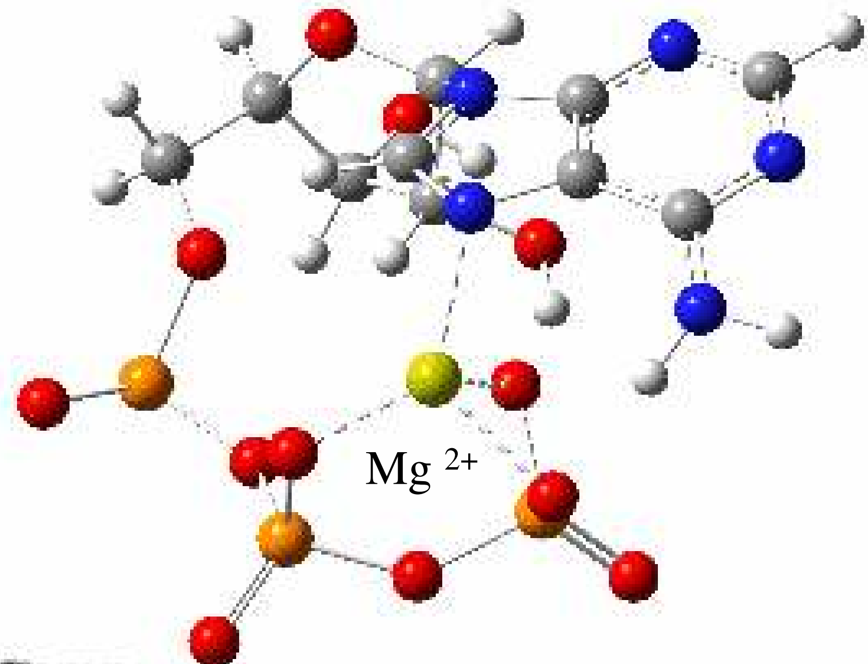
$$[AT\Phi] = \frac{k_T(k_{ST}+k_S)}{k_{ST}(k_T+k_{-1})+k_T(k_S+k_{-1})} = \left(1+\frac{k_{-1}(k_{ST}+k_T)}{k_T(k_{ST}+k_S)}\right)^{-1}.$$

$$k_T > k_S$$

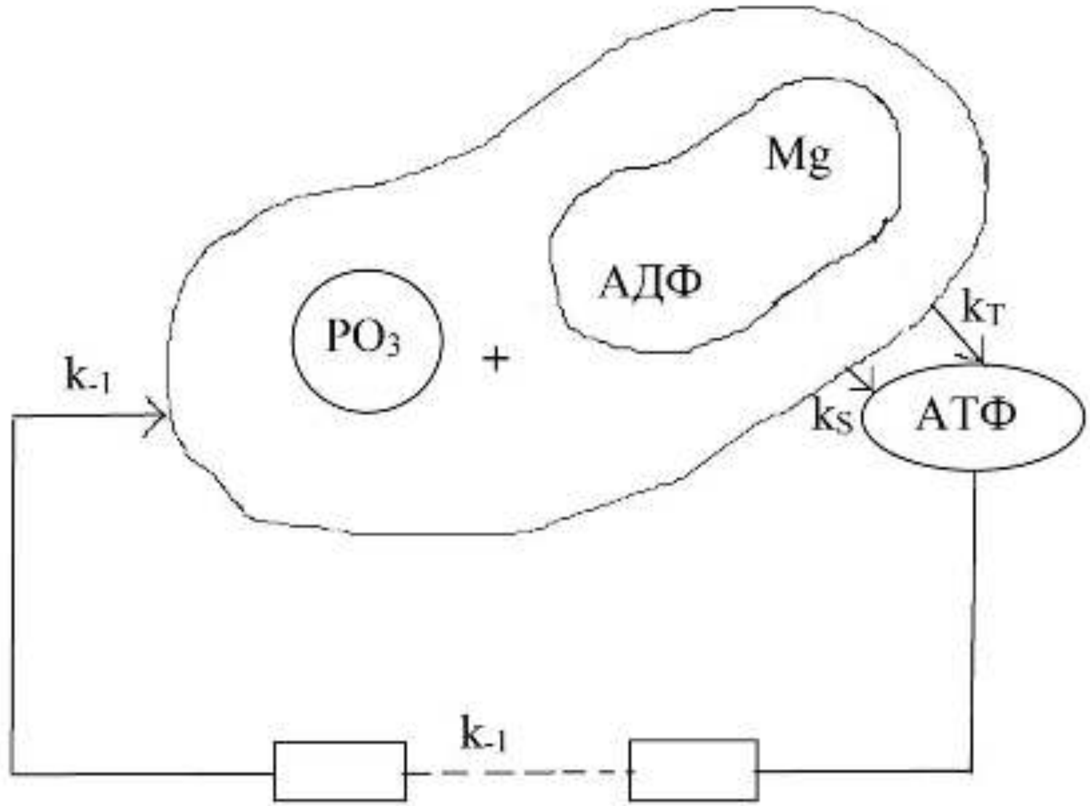
ATP and complex Mg-ATP







Scheme of intracellular enzymatic synthesis and consumption of ATP



$$\left[(Mg - АДФ)^{S,T} + PO_3^{-}\right] \xrightarrow{k_S, k_T} (АТФ)$$

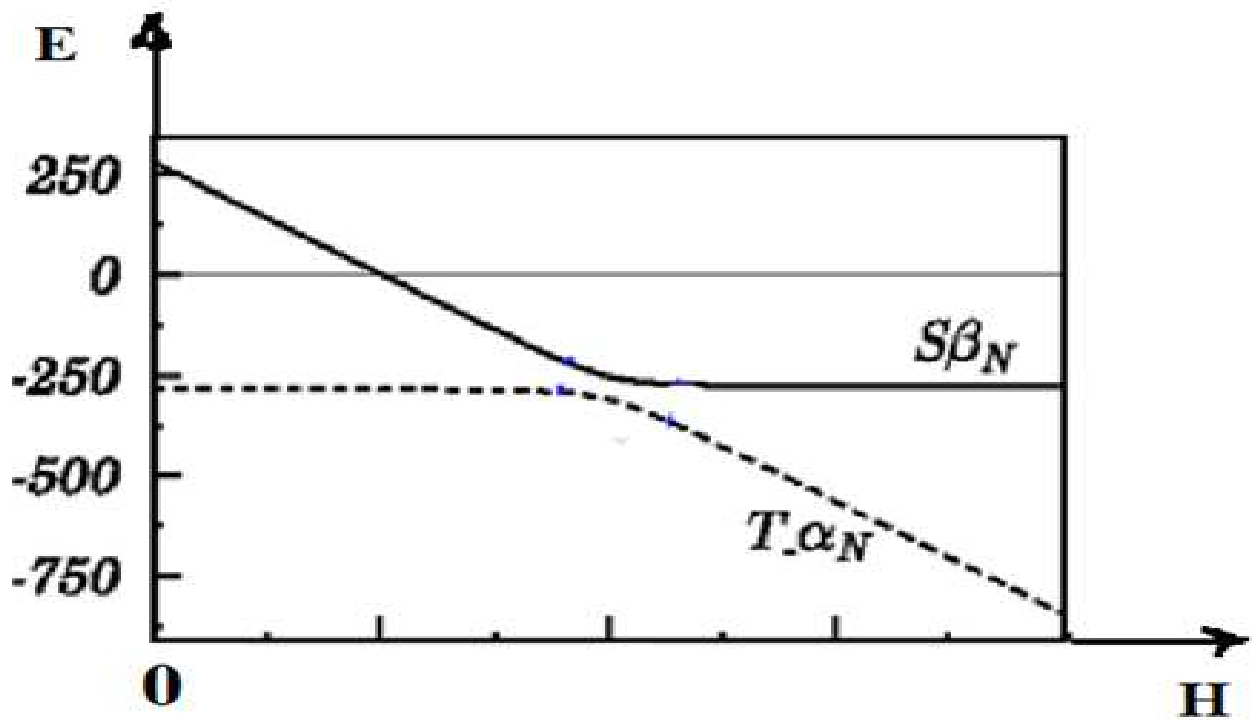
k_{-1}

The effect of Mg nuclear spin on ATP synthesis in strong magnetic fields

Spin Hamiltonian of two indistinguishable electrons in molecules

$$H = g\beta \mathrm{H}(S_1 + S_2) + J\vec{S}_1\vec{S}_2 + a(S_1 - S_2)\vec{I}$$

Graph of the energy dependence on the magnetic field in the area of intersection of S-T-terms



The effect of Mg nuclear spin on ATP synthesis in strong magnetic fields

$$\frac{d\rho}{dt} = -ih^{-1}[H,\rho] - \frac{k_S}{2}\{P_S\rho + \rho P_S\} - \frac{k_T}{2}\{P_T\rho + \rho P_T\} + k_{-1}|S\rangle\rho_C\langle S|,$$

$$\frac{d\rho_C}{dt} = k_S P_S \rho P_S + k_T \rho P_T - k_{-1}\rho_C$$

$\rho(t)$ – матрица плотности комплексов [Mg–АДФ, $PO_3]^{S,T}$,

$\rho_C(t)$ – матрица плотности диамагнитных молекул АТФ,

P_S – оператор проектирования в S состояние электронном пары,

P_T – оператор проектирования в T состоянии электронной пары.

ATP yield

$$\rho_C(\mathrm{H}) = \frac{k_S}{k_S + k_{-1}} + \frac{k_{-1}}{k_T} \cdot \frac{(k_T^2 - k_S^2)}{(k_S + k_{-1})^2} \cdot \frac{a^2}{\omega^2 + k_{ST}^2 + a^2 \dfrac{(k_S + k_T)\cdot(k_S + k_T + 2k_{-1})}{k_T(k_S + k_{-1})}}$$

Magnetic field dependence of ATP yield

$$\rho_C(\mathrm{H}) = \frac{k_S}{k_S + k_{-1}} + \frac{k_{-1}}{k_T} \cdot \frac{(k_T^2 - k_S^2)}{(k_S + k_{-1})^2} \cdot \frac{a^2}{\omega^2 + k_{ST}^2 + a^2 \dfrac{(k_S + k_T)\cdot(k_S + k_T + 2k_{-1})}{k_T(k_S + k_{-1})}}$$

It is the Lorenz function with centre $\omega = g\beta H - J = 0$

Width

$$\Delta\omega_{1/2} = 2\sqrt{k_{ST}^2 + a^2 \frac{(k_S + k_T)\cdot(k_S + k_T + 2k_{-1})}{k_T(k_S + k_{-1})}}$$

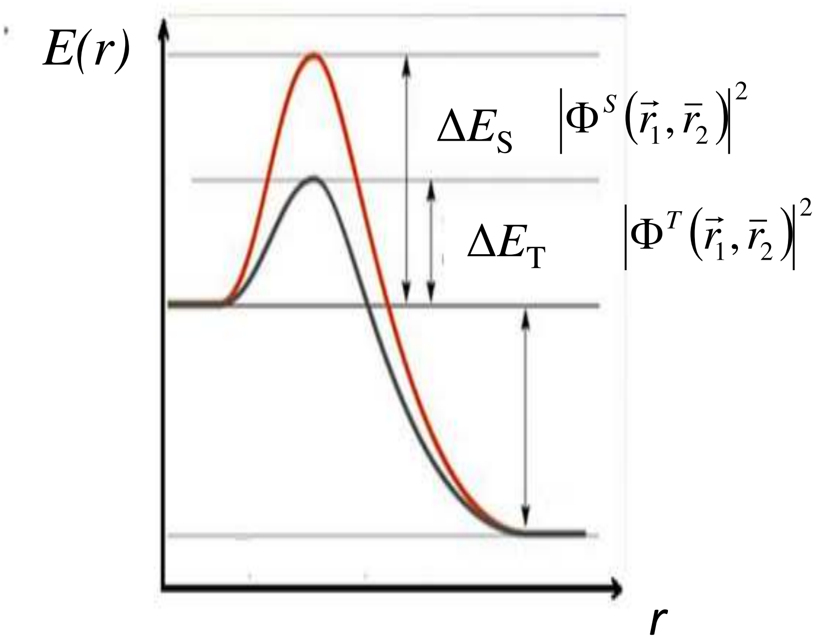
Amplitude

$$\Delta\rho(\omega_0) = a^2 \frac{k_{-1}}{k_T} \cdot \frac{(k_T^2 - k_S^2)}{(k_S + k_{-1})^2} \cdot \frac{1}{(\Delta\omega_{1/2})^2}$$

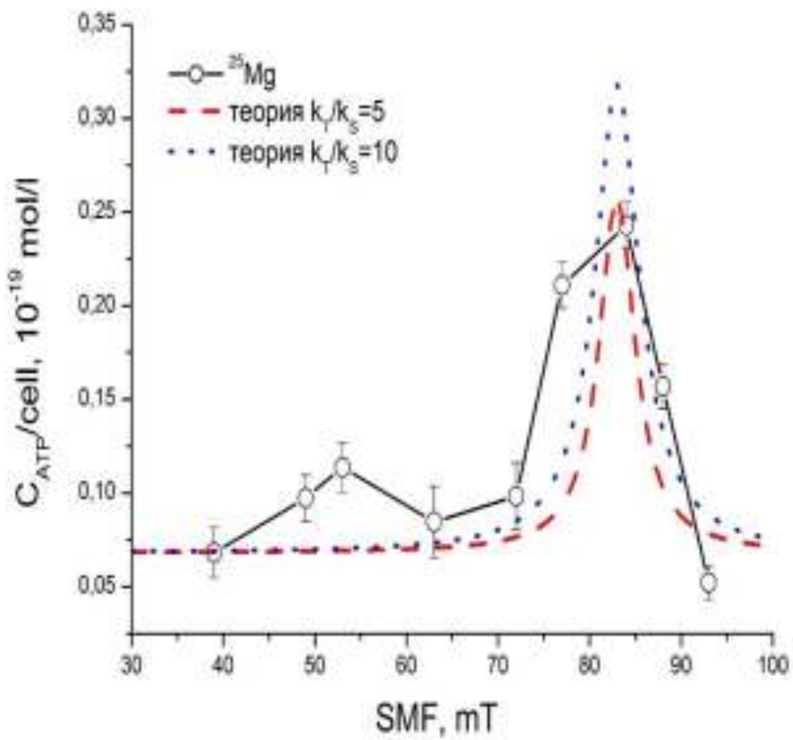
S-T conversion and electron density $\left|\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2)\right|^2$ redistribution

$$\left\langle \Psi^T(\vec{r}_1, \vec{r}_2, s) \middle| \widehat{H}_F \middle| \Psi^S(\vec{r}_1, \vec{r}_2, s) \right\rangle = \left\langle T_{0,\pm} \middle| \left\langle \Phi_r^T(\vec{r}_1, \vec{r}_2) \middle| \widehat{H}_F \middle| \Phi_r^S(\vec{r}_1, \vec{r}_2) \right\rangle \middle| S \right\rangle$$

Potential energy *E(r)* of reagents



Calculated MF dependence of ATP yield



Effects of magnetic field and nuclear spin on rate of ATP synthesis

Conclusions

- Hyperfine interaction $a(\vec{S}_1 - \vec{S}_2)\vec{I}$ of paired electrons induces spin S-T conversion in diamagnetic complexes Mg-ADP
- Spin S-T conversion is accompanied by redistribution of electron densities $\left|\Phi^S(\vec{r}_1, \vec{r}_2)\right|^2$ in Mg-ADP complexes.
- Redistribution of electron densities decreases Coulomb repulsion and activation energy of ATP synthesis via reaction $\mathrm{ADP}^{(-)} + \mathrm{PO}_3^-$
- Spin S-T conversion and redistribution of electron densities increase the rate of intracellular enzymatic synthesis and ATP yield *in vivo*.