THEORETICAL CALCULATIONS OF THE ENERGY BALANCE OF ATP SYNTHASE GAMMA-SUBUNIT ROTATION

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The FoF1 ATP synthase molecular motor synthesizes ATP from ADP and phosphate (Pi) in cells. Most researchers believe that the ATP synthase consists of two motors, where the rotors of both the motors are constructively linked with each other and rotate jointly in opposite directions depending on the using energy source. The F1 complex (comprising subunits α3, β3, γ, ε and δ) is a rotary mechano-chemical motor powered by ATPase activity and is composed of an axle (the γ-subunit) that rotates within its (αβ)3-ring stator. The (αβ)3-ring, with a catalytic site located between three α- and β-subunits, surrounds the γ-subunit coiled-coil domain. The adjacent γ-"foot" domain docks to the c-ring of c-subunits in Fo. The membrane-embedded electric motor – Fo (the proton transporting c-ring and a, b2 subunits) utilizes energy of the electrochemical potential - ΔμH+ as an energy source to rotate the c-ring in the opposite direction from that powered by the F1 motor. However, we do not agree that Fo is an electric motor and offer a mechano-chemiosmotic mechanism of ATP synthesis. According to our model ATP synthase is a Ca2+/H+- K+ Cl- -pump-pore-enzyme complex, in which γ-subunit rotates 360o in steps of 30o, and 90o due to the binding of phosphate ions to positively charged amino acid residues in the N-terminal γ-subunit, while in the electric field. In order to evaluate the energy efficiency of such twisting we calculated the energy balance in binding phosphate ions to protonated residues of arginine and lysine. The energy of binding equal to 0.00 kcal/mol in the base state and 4.39 kcal / mol after phosphatization of the protonated groups at a value equal to the dielectric constant of 61. Negative energy figure shows the stability of the system, and a positive value on the implementation of the positive work in which energy is decreasing waning. Our calculations show a hyperbolic dependence of the interaction energy on the dielectric constant. Obviously, the dielectric constant in this case, indicates the amount of water in the matrix. ATP is then synthesized during the reverse rotation of the γ-subunit by destabilizing the phosphated N-terminal γ-subunit and b2- subunits under the influence of Ca2+ ions, which are pumped over from storage - intermembrane space, during swelling of organells. [A link to the animation: http://www.youtube.com/watch?v=PgKoKnVvBi4].