## Definitions

Relations
Laws and Values
A. $\mathrm{H}_{2} \mathbf{O}-\mathrm{H}^{+}$- the high-energy source of $\mathrm{H}^{+}$:
$\Delta \mathrm{E}_{1}$ - free energy of $\mathrm{H}_{2} \mathrm{O}-\mathrm{H}^{+}$in water.
$\mathrm{Ek}\left(\mathrm{H}^{+}\right), \mathrm{M}\left(\mathrm{H}^{+}\right), \mathrm{V}\left(\mathrm{H}^{+}\right)$, - kinetic energy, mass, and velocity of $\mathrm{H}^{+}$.
$\Delta \mathrm{E}_{2}$-heat of evaporation-condensation. $\Delta \mathrm{E}_{3}$-heat of acid-base neutralization. $\Delta \mathrm{E}_{4}$ - the free energy of ATP hydrolysis $\Delta \mathrm{E}_{5}$ - the enthalpy of ATP hydrolysis in closed cycles of muscle contraction.
$\lambda$ - de-Broglie wavelength of $\mathrm{H}^{+}$.
B. Dimer's spin (s) and precession (p): Ed - the binding energy between dimers Es, Ls, Is - the dimer spin kinetic energy, angular momentum and moment of inertia.
$\mathrm{R}(\mathrm{H} 1), \mathrm{R}(\mathrm{H} 2)-$ spinning radiuses of the dimer two pairs of bound protons.
$\mathrm{Mp}, \mathrm{Mw}$ - proton and water molecule mass. $\mathrm{Ld}, \mathrm{Dd}, \mathrm{Nd}$ - the length, width and volume of dimer occupation in liquid water, assuming 2 lengthwise and 4 anti-parallel neighbors.
Dw - effective diameter of a water molecule Dwp, Vwp, Ewp - the water molecule precession diameter, velocity and energy. fdp, Ldp, Edp - the dimer's precession frequency, angular momentum, and energy fmw, Emw - microwave frequency and energy.
All values are related to the higher state of dimer precession.

## C. The soliton's dimensions:

$\mathrm{L}\left(\mathrm{H}^{+}\right), \mathrm{t}\left(\mathrm{H}^{+}\right)-\mathrm{H}^{+}$flight length and duration. Ns - number of water molecules per soliton. Ms, v, $\rho$, Rs, Ls - soliton's mass, volume, density, radius and length.
$\mathrm{Nd} / \mathrm{r}, \mathrm{Nr} / \mathrm{s}$ - number of dimers per ring, and number of rings per soliton.

## D. The soliton hydraulic action:

$\Delta \mathrm{E}, \Delta \mathrm{Po}, \nabla \mathrm{P}, \mathrm{Fs}$ - the soliton's energy, pressure-head, pressure-gradient, force, $\mathrm{Fp}(\mathrm{r}), \mathrm{Ft}(\mathrm{r}), \mathrm{T}(\mathrm{r})$, $\mathrm{Vf}(\mathrm{r})$ - pressure-head force, tangential motive force, shearing stress, and effective flow velocity of AS, at radius $r \leq$ Rs. $\eta$, FRs - water viscosity and soliton flow rate. Vs, $\tau$ - the soliton's translation velocity and propelling duration across $\Delta \mathrm{Po}$, in absence of external work production.
V1s, H1s, f1s - velocity per unit length, power and shearing factor per unit volume.

HR1s - the hydrolytic-rate per unit volume of the A-M ATPase, corresponding to H1s.
E. Solitons in a half sarcomere (hs):

Fhso - the isometric hydraulic force in sarcomere compression.
Lhs, Ahs, Vhso, Nhs - length, cross-section area, unloaded shortening velocity, and volume of a half sarcomere.
V1o, H1o, f1 - velocity per unit length, power and shearing force factor per unit volume for a half sarcomere, at unloaded contraction.

These relations are applied for the quantitative formulation of muscle contraction (Box3).

$$
\begin{aligned}
& {\left[\mathrm{H}_{2} \mathrm{O}-\mathrm{H}^{+}\right] /\left[\mathrm{H}_{2} \mathrm{O}\right]=\operatorname{EXP}\left\{-\Delta \mathrm{E}_{1} / \mathrm{kT}\right\}} \\
& \mathrm{Ek}\left(\mathrm{H}^{+}\right)=\Delta \mathrm{E}_{1} \\
& \mathrm{~V}\left(\mathrm{H}^{+}\right)=\left(2^{*} \operatorname{Ek}\left(\mathrm{H}^{+}\right) / M\left(\mathrm{H}^{+}\right)\right)^{1 / 2} \\
& \Delta \mathrm{E}_{1}=\Delta \mathrm{E}_{2}=\Delta \mathrm{E}_{3}=\Delta \mathrm{E}_{4}=\Delta \mathrm{E}_{5}=\Delta \mathrm{E} \\
& \boldsymbol{\lambda}=\mathrm{h} /\left(\left(\mathrm{M}\left(\mathrm{H}^{+}\right)^{\star} \mathrm{V}\left(\mathrm{H}^{+}\right)\right)\right. \\
& -E d=\Delta E=2 * E s \\
& E s=L s^{2} /\left(2^{*} \mid s\right) \\
& R(\mathrm{H} 1)=\mathbf{2}^{\star} \mathrm{R}(\mathrm{H} 2) \\
& \begin{array}{c}
R(\mathrm{H} 1)=2^{\star} \mathrm{R}(\mathrm{H} 2) \\
\text { Is }=2^{\star} \mathrm{Mp} \mathrm{p}^{\star}\left(\mathrm{R}(\mathrm{H} 1)^{2}+\mathrm{R}(\mathrm{H} 2)^{2}\right)=10^{\star} \mathrm{Mp}{ }^{\star} \mathrm{R}(\mathrm{H} 2)^{2}
\end{array} \\
& \text { Ls }=\left(2^{\star} \mid s^{*} E s\right)^{1 / 2}=\left(20^{\star} \mathrm{Mp}^{\star} R(\mathrm{H} 2)^{2} \mathrm{Es}\right)^{1 / 2} \\
& \begin{array}{c}
M p=1 / A \# g r, M w=18 / A \# g r \\
\left(A \#=6.022^{\star} 10^{23}-\right.\text { Avogadro's \#) }
\end{array} \\
& \mathrm{Nd}=\mathrm{Ld}^{*}(\mathrm{Dd})^{2}=2^{*} 18 / A \# \mathrm{~cm}^{3} \\
& \text { Dwp = Dd - Dw } \\
& M w=18 / A \# g r \\
& \text { Ldp }=2^{*} \mathrm{Mw}^{*} \text { Vwp*Dwp/2 }=\hbar \\
& \text { Vwp }=\hbar /\left(M w^{\star} \text { Dwp }\right), \quad \text { Ewp }=1 / 2^{*} \mathbf{M w}^{\star} \text { Vwp }{ }^{2} \\
& E d p=2^{\star} E w p, E d p=E m w=h^{\star} f d p
\end{aligned}
$$

$t\left(H^{+}\right)=1 / \mathrm{fmw}$
$\mathrm{L}\left(\mathrm{H}^{+}\right)=0.5^{\star} \mathrm{V}\left(\mathrm{H}^{+}\right)^{\star} \mathrm{t}\left(\mathrm{H}^{+}\right)$
$\mathrm{Ns}=\Delta \mathrm{E} / \mathrm{Ewp}=\mathrm{Ms} / \mathrm{Mw}$
Ms $=\mathrm{Ns}^{\star} \mathrm{Mw}=\mathbf{v}^{\star} \rho$
$v=\pi^{*}$ Rs $^{2}{ }^{*} L s, L s=L\left(H^{+}\right)$
Rs $=\left[\mathbf{v} /\left(\pi^{*} L s\right)\right]^{1 / 2}$
$\mathrm{Nr} / \mathrm{s}=0.5^{*} \mathrm{Ns} / \mathrm{Nd} / \mathrm{r}$

Fs $=\pi^{\star} \operatorname{Rs}^{2}{ }^{\star} \Delta P=\pi^{\star} R^{2}{ }^{\star} L^{*} \Delta P / L=v^{\star} \nabla P$
$\Delta E=\int v^{\star} \nabla P^{\star} d l=v^{\star} \Delta P o$
Thus: $\Delta \mathrm{Po}=\Delta \mathrm{E} / \mathrm{v}$ $\mathrm{Ft}(\mathrm{r})=\mathrm{Fp}(\mathrm{r})$
$\mathrm{T}(\mathrm{r})^{\star} 2 \pi^{\star} \mathrm{r}^{\star} \mathrm{L}=\Delta \mathrm{Po}^{\star} \pi^{\star} r^{2}$
$T(r)=1 / 2^{*} \Delta \mathrm{Po} / L^{*} r=k^{*} r$
$T(r)=-\eta^{*} d V f(r) / d r$
$V f(r)=\int d V f(r)=k / \eta^{*}\left(R^{2}-r^{2}\right)$
FRs $=\int \mathrm{Vf}(\mathrm{r})^{\star} 2 * \pi^{\star} \mathrm{r}^{\star} \mathrm{dr}=\mathrm{k} /(2 \eta)^{\star} \pi^{\star} \mathrm{Rs}^{4}$
$=\Delta \mathrm{Po}^{\star} \pi^{\star} \mathrm{Rs}^{4} /\left(4^{\star} \eta^{\star}\right.$ Ls $)$
$\tau=\mathrm{v} / \mathrm{FRs}=\mathrm{Ls} / \mathrm{Vs}=1 / \mathrm{V} 1 \mathrm{~s}$
$\mathrm{H} 1 \mathrm{~s}=(\Delta \mathrm{E} / \mathrm{v}) / \tau=\Delta \mathrm{Po} / \tau=\Delta \mathrm{Po}^{*} \mathrm{~V} 1 \mathrm{~s}$
$\mathrm{f} 1 \mathrm{~s}=\mathrm{H} 1 \mathrm{~s} / \mathrm{V} 1 \mathrm{~s}^{2}=\Delta \mathrm{Po}^{\star} \tau=\Delta \mathrm{Po} / \mathrm{V} 1 \mathrm{~s}$

$$
H R 1 s=H 1 s / \Delta E
$$

$$
\text { Fhso }=\Delta \mathrm{Po}^{\star} \text { Ahs }=\Delta \mathrm{Po}^{\star} \mathrm{Nhs} / \text { Lhs }
$$

Vhs $(\max )=\mathrm{V} 10(\max )^{\star}$ Lhs $=\mathrm{V} 1 \mathrm{~s}^{\star}$ Ls $=\mathrm{Vs}$

## H1o(max)*Lhs = H1s*Ls

$\Delta \mathrm{Po}=\mathrm{f} 1 * \mathrm{~V} 10(\max )=\mathrm{f} 1 \mathrm{~s}^{*} \mathrm{~V} 1 \mathrm{~s}$
Therefore: $\mathrm{H} 1 \mathrm{~s} / \mathrm{H} 10(\max )=$
$=$ V1s/V1o $($ max $)=\mathrm{f} 1 / \mathrm{f} 1 \mathrm{~s}=$ Lhs/Ls
The same value of $f 1$ is related in general to striated muscle contraction, therefore: $\mathrm{f} 1{ }^{*} \mathrm{~V} 10(\mathrm{max})=\mathrm{Po}=1000 \mathrm{grwt} / \mathrm{cm}^{\wedge} 2$ H10 = f1*V10^2

The Maxwell - Boltzmann relation.
$\Delta \mathrm{E}_{1}=-\mathrm{kT} \mathrm{K}^{*} \ln \left[10^{-7} / 55.6\right]=20^{*} \mathrm{kT}$
(at $290^{\circ} \mathrm{K}, \mathrm{kT}=0.4^{*} 10^{-13}$ ergs)
$\mathrm{V}\left(\mathrm{H}^{+}\right)=10^{6} \mathrm{~cm} / \mathrm{sec}=10 \mathrm{~km} / \mathrm{sec}$
$\Delta \mathrm{E}=0.8^{*} 10^{-12}$ ergs $=0.5$ proton ${ }^{*}$ volt $=$ $=11.5 \mathrm{kcal} / \mathrm{mole}=48 \mathrm{kJoule} / \mathrm{mole}$
$\lambda=0.4^{\star} 10^{-8} \mathrm{~cm}$

The virial theorem.
Es $=0.4^{\star} 10^{-12} \mathrm{erg}, \mathrm{Mp}=1.67^{\star} 10^{-24} \mathrm{gr}$
$R(\mathrm{H} 1)=2^{*} R(\mathrm{H} 2)=1.4^{*} 10^{-8} \mathrm{~cm}$ (Fig.1a)
Ls $=25.6^{\star} 10^{-27} \mathrm{erg}^{\star} \mathrm{sec} \approx 25^{\star} \hbar$
$\mathrm{Nd}=6^{\star} 10^{-23} \mathrm{~cm}^{3}, \mathrm{Ld}=4.2^{\star} 10^{-8} \mathrm{~cm}$
Dd $=3.8^{\star} 10^{-8} \mathrm{~cm}, \mathrm{Dw} \approx 1.3^{\star} 10^{-8} \mathrm{~cm}$
Dwp $=2.5^{\star} 10^{-8} \mathrm{~cm}$
$\mathrm{Mw}=3^{*} 10^{-23} \mathrm{gr}$
Vwp $=1.4^{*} 10^{3} \mathrm{~cm} / \mathrm{sec}$
Ewp $=3^{*} 10^{-17}$ ergs
Edp $=E m w=6^{\star} 10^{-17}$ ergs
$\mathrm{fdp}=\mathrm{fmw} \approx 10^{10}$ cycles $/ \mathrm{sec}$
$\mathrm{t}\left(\mathrm{H}^{+}\right)=10^{-10} \mathrm{sec}$
$\mathrm{L}\left(\mathrm{H}^{+}\right)=0.5^{\star} 10^{-4} \mathrm{~cm}=0.5 \mu \mathrm{~m}$
Ns $=26768$ water molecules, $\rho=1 \mathrm{gr} / \mathrm{cm}^{3}$
Ms $=0.8^{\star 1} 0^{-18} \mathrm{gr}, \mathrm{v}=0.8^{\star} 10^{-18} \mathrm{~cm}^{3}$
$L s=5^{*} 10^{-5} \mathrm{~cm}=500 \mathrm{~nm}$
Rs $=7^{*} 10^{-8} \mathrm{~cm}=0.7 \mathrm{~nm}$
$\mathrm{Nd} / \mathrm{r}=8, \mathrm{Nr} / \mathrm{s}=1673$

A general version of Archimedes Law.
Bernoulli's Equation.
$\Delta \mathrm{Po}=10^{6} \mathrm{erg} / \mathrm{cm}^{3}=0.1 \mathrm{Joule} / \mathrm{cm}^{3}=$

$$
=10 \text { Newton } / \mathrm{cm}^{2} \approx 1 \mathrm{kgwt} / \mathrm{cm}^{2}
$$

Balance between the shearing force of AS and the opposing pressure-head force.
Newton's Stress-Viscosity Relation.
Active version of Poiseuille's Law.
$\eta=10^{-2}$ Poise $=1 \mathrm{cP}\left(\right.$ at $20^{\circ} \mathrm{C}$ )
FRs $=4^{*} 10^{-17} \mathrm{~cm}^{3} / \mathrm{sec}$
$\tau=20 \mathrm{msec}$
$\mathrm{V} 1 \mathrm{~s}=50 \mathrm{sec}^{-1}, \mathrm{Vs}=25 \mu \mathrm{~m} / \mathrm{sec}$
$\mathrm{H} 1 \mathrm{~s} \approx 5^{*} 10^{7} \mathrm{erg} / \mathrm{sec} / \mathrm{cm}^{3}=5$ Watt $/ \mathrm{cm}^{3}$
$\mathrm{f} 1 \mathrm{~s} \approx 2 \mathrm{~mJ} \mathrm{Jec}^{*} / \mathrm{cm}^{3}$
HR1s $\approx 100$ ( $\mu$ mole ATP) $/ \mathrm{cm}^{3} / \mathrm{sec}$

## $\Delta P o$ is independent of HR.

Fhso is proportional to Ahs.

## Lhs/ Ls $\approx 2$

Vhs(max) $=\mathrm{Vs}=\mathbf{2 5} \mu \mathrm{m} / \mathrm{sec}$;
$\mathrm{V} 1 \mathrm{o}(\max ) \approx 25 \mathrm{sec}^{-1} ;\left(\right.$ at $20^{\circ} \mathrm{C}$ )
$\mathrm{H} 10(\max ) \approx 2.5 \mathrm{~W} / \mathrm{cm}^{3}$;
$\mathrm{f} 1 \approx 2^{\star} \mathrm{f} 1 \mathrm{~s}=4 \mathrm{~mJ} / \mathrm{cm}^{3 *} \mathrm{sec}$
$=40$ grwt $^{\star} \mathrm{cm} / \mathrm{cm}^{3 *} \mathrm{sec}$
$\mathrm{H} 1 \mathrm{o} \approx 4^{\star} \mathrm{V} 1 \mathrm{o}^{2} \mathrm{~mW} / \mathrm{cm}^{3}$ ( at $20^{\circ} \mathrm{C}$ )

Box 2. Heat contributions due to elastic and baro-entropic components in a half sarcomere

| Definitions |  |
| :--- | :--- |

1. Huxley, A.F.; Tideswell, S. Filament compliance and tension transients in muscle. J. Muscle Res. Cell Motil. 1996, 17(4), 507-511.
2. Abbot, B.C.; Baskin, R.J. Volume changes in frog muscle during contraction. J. Physiol. 1962, 161,379391.
3. Gilbert, C.; Kretzschmar, K.M.; Wilkie, D.R.; Woledge, R.C. Chemical change and energy output during muscular contraction. J. Physiol. 1971, 218, 163-193..
4. Canfield, P.; Lebacq, J.; Marechal, G. Energy balance in frog sartorius muscle during an isometric tetanus at 20 degrees C. J. Physiol. 1973, 232, 467-483.

Box 3. Mechano-chemical conversion into hydraulic compression by active streaming in isotonic and
isometric contractions ( Fig.3; Interactive Workbook 1) isometric contractions ( Fig.3; Interactive Workbook 1)

| Definitions | Relations |
| :---: | :---: |
| I. A. The power-balance and force-velocity relations <br> J. (for a half sarcomere of $1 \mu \mathrm{~m}$ at $20^{\circ} \mathrm{C}$ ) ${ }^{*}$ : <br> $\mathrm{Hm}^{\prime}, \mathrm{Hq}^{\prime}, \mathrm{Hh}$ - mechanical, heat and hydrolytic power components. $\mathrm{u}, \mathrm{e}$ - rate, and mechano-chemical energy, of ATP hydrolysis. <br> $\mathrm{Ht}^{\prime}$, Hc - heat components due to translation and circulation of AS. <br> $\mathrm{Vt}^{\prime}$, Vc' - flow velocity of the translation and circulation of AS. <br> $\mathrm{V}^{\prime}=\mathrm{Vt}^{\prime}, \mathrm{F}^{\prime}$ - shortening velocity and the hydraulic force. <br> $\mathrm{Ft}^{\prime}=\mathrm{f}^{\star} V \mathrm{Vt}^{\prime}, \mathrm{Fc}^{\prime}=\mathrm{g}^{*} V c^{\prime}-$ fluid shearing forces related to $\mathrm{Vt}^{\prime}$ and $\mathrm{Vc}^{\prime}$. <br> $\mathrm{L}, \mathrm{A}, \mathrm{N}$ - length, cross-section area and volume. <br> V1, P1, H1 - velocity, force, power, per unit of length, area, volume. <br> $\mathrm{V} 10, \mathrm{P} 10, \mathrm{H} 10$ - the above unloaded and isometric values. <br> $\mathrm{V}, \mathrm{P}, \mathrm{H}$ - the variables normalized by the isometric values. <br> * Note that no account is made for the expansion effect and for viscosity changes with temperature. |  |
| B. The Fenn Effect inclusion: <br> The Fenn Effect was revealed as an increase of Hh in linear proportion to Hm . Theoretically, this effect is predicted by a decrease in the soliton lifetime upon external energy transfer. Thus, a change in Hm induces equal but opposite changes in both Hh and Hq , relative to $\mathrm{Ho}=\mathrm{Hho}=\mathrm{Hqo}=1$. This argument leads to the differential and integral relations of the Fenn Effect. <br> As presented and enacted in the attached Microsoft Excel workbook, The $\mathrm{P}-\mathrm{V}$ profile for a given value of $\mathbf{a}$, is obtained by taking the variable parameter Hm in steps from zero to its optimum value Hmop, and down to zero. Thus, Eq. 3 enables to construct the P-V profiles of isotonic contractions (Fig. $3 \mathrm{~A}, \mathrm{~B}$ ), isometric tetanus, and twitch contractions (Section C, Fig. 3 C, D)). It further enables a theoretical evaluation of the phenomenological force-velocity relation of A. V. Hill. | The differential relation for the Fenn Effect: <br> $\mathrm{dHh} / \mathrm{dHm}=-\mathrm{dHq} / \mathrm{dHm}$ <br> Apply Eq. 2 on Eq. 1 to get the integral Fenn Effect relation: $\mathrm{Hh}=1+\mathrm{Hm} / 2, \mathrm{Hq}=1-\mathrm{Hm} / 2$ <br> (2') <br> Substitute $\quad \mathrm{Hh}=1+0.5^{*} \mathrm{a}^{*} \mathrm{P}^{\star} \mathrm{V}$ in equation (1'), to get: $\begin{equation*} a^{*} P^{*} V+V^{2}+P^{2}=1+0.5^{*} a^{*} P^{*} V \tag{3} \end{equation*}$ <br> Substitute $\quad P=H m /\left(a^{*} V\right)$ to get: $\begin{equation*} v^{4}-b^{\star} V^{2}+c=0 \tag{3'} \end{equation*}$ <br> Where $b=1-\mathrm{Hm} / 2 ; c=(\mathrm{Hm} / \mathrm{a})^{2}$ <br> By symmetry, the solution of Eq.(3') for a given Hm and a is: $\begin{equation*} \left(V^{2}\right)_{1,2}=\left(\mathbf{P}^{2}\right)_{2,1}=\mathrm{b} / 2 \pm\left((\mathrm{b} / 2)^{2}-\mathrm{c}\right)^{1 / 2} \tag{3'’} \end{equation*}$ <br> At optimum : $\begin{gathered} \text { Pop = Vop, } \quad(b / 2) \text { op }=\text { Hmop/a } / a \\ \text { Hmop }=2^{\star} \mathrm{a} /(\mathrm{a}+4)=\mathrm{a}^{*} \mathrm{Pop}^{2} \\ \text { Pop }=(2 /(\mathrm{a}+4))^{1 / 2} \\ \mathrm{a}=2 / \mathrm{Pop}^{2}-4 \end{gathered}$ |
| C. Isometric contractions against elastic elements: <br> Tetanus (Fig. 3 C of the manuscript): <br> $\mathrm{C}^{\prime}$, C1, C - compliance, compliance per unit cubic volume of muscle, and the normalized compliance. <br> Em, Eq, Eh - Normalized mechanical, heat, and input energy. These values are obtained by numerical integration of successive isotonic states, as presented in the attached workbook (Suppl Workbook 1). To, Eo - the units of time and energy, defined by V1o and H1o. <br> Twitch (Fig. 3 D): <br> $C(P, N(t)=1)$ - The load-normalized compliance for twitch contraction that develops the tension P , during the time t , when the AS circulation, Vs, just spans the whole sarcomere volume. This total circulation flow is presumed to allow for peripheral effective depletion of calcium ions by the sarcoplasmic reticulum. | $\begin{equation*} \mathrm{dL}^{\prime}=\mathrm{C}^{\prime} \mathrm{dF}^{\prime}=>\mathrm{V}^{\prime}=\mathrm{C}^{\prime *} \mathrm{dF} / \mathrm{dt}^{\prime} \tag{4} \end{equation*}$ <br> The normalized formula is: $\mathrm{dL} / \mathrm{dt}=\mathrm{V}=\mathrm{C}^{*} \mathrm{dP} / \mathrm{dt}$ <br> Where: $\mathrm{dL}=\mathrm{dLL}^{\prime} / \mathrm{Lo}, \mathrm{V}=\mathrm{V}^{\prime} / \mathrm{V}^{\prime} \mathrm{o}=\mathrm{V} 1 / \mathrm{V} 10 ; \mathrm{F}=\mathrm{F}^{\prime} / \mathrm{Fo}^{\prime}=\mathrm{P}^{\prime} / \mathrm{Po}=\mathrm{P}$; $\mathrm{C} 1=\mathrm{C}^{\prime *} \mathrm{Ao} / \mathrm{Lo}=\mathrm{dL} / \mathrm{dP}{ }^{\prime} ; \mathrm{C}=\mathrm{C} 1 * \mathrm{Po} ; \mathrm{dt}=\mathrm{dt} / \mathrm{to} ; \mathrm{to}=1 / \mathrm{V} 1 \mathrm{o} ; \mathrm{Eo}=\mathrm{H} 1 \mathrm{o}^{*}$ to $\begin{equation*} \mathrm{dEm} / \mathrm{dt}=\mathrm{Hm}=>\mathrm{dt}=\mathrm{dEm} / \mathrm{Hm} \tag{5} \end{equation*}$ $\begin{equation*} E m(t)=\int H m^{*} d t=\int a^{*} V^{*} P^{*} d t=\int a^{*} C^{*} d P / d t{ }^{*} P^{*} d t=0.5^{*} a^{*} C^{*} P(t)^{2} \tag{6} \end{equation*}$ $\begin{equation*} \mathrm{Eq}(\mathrm{t})=\int \mathrm{Hq}^{*} \mathrm{dt}=\int(1-\mathrm{Hm} / 2)^{*} \mathrm{dt}=\mathrm{t}-\mathrm{Em}(\mathrm{t}) / 2 \tag{7} \end{equation*}$ $\begin{equation*} \mathrm{Eh}(\mathrm{t})=\int \mathrm{Hh}^{\star} \mathrm{dt}=\int(1+\mathrm{Hm} / 2)^{\star} \mathrm{dt}=\mathrm{t}+\mathrm{Em}(\mathrm{t}) / 2 \tag{7'} \end{equation*}$ <br> Twitch condition: $\mathrm{N}(\mathrm{t})=\mathrm{VV} s^{*} \mathrm{dt}=1, \quad$ where: $\mathrm{V} \mathrm{s}=(\mathrm{Hh})^{1 / 2}$ |

Table 1.Molecular distances in a pair of dimers (Fig.1A)

|  | $\begin{aligned} & \hline \mathrm{O} 12- \\ & \mathrm{H} 12 \\ & \hline \end{aligned}$ |  | $\begin{array}{\|l\|} \hline \text { O11- } \\ \text { H11 } \\ \hline \end{array}$ |  |  | $\begin{aligned} & \mathrm{O} 12- \\ & \mathrm{H} 21 \\ & \hline \end{aligned}$ | $\begin{aligned} & \hline \text { O11- } \\ & \text { H12 } \\ & \hline \end{aligned}$ |  |  |  | $\begin{aligned} & \hline \mathrm{O} 11- \\ & \mathrm{H} 21 \\ & \hline \end{aligned}$ |  |  | $\begin{aligned} & \text { O11- } \\ & \text { H22 } \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| OH | 1 |  | 2 |  |  | 3.16 | 3.61 |  |  |  | 5.83 |  |  | 7.81 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  | $\begin{aligned} & \hline \text { O12- } \\ & \mathrm{O} 21 \\ & \hline \end{aligned}$ |  |  | $\begin{aligned} & \text { O11- } \\ & 012 \end{aligned}$ |  |  | $\begin{aligned} & \mathrm{O} 11- \\ & \mathrm{O} 21 \end{aligned}$ |  |  |  |  | $\begin{aligned} & \text { O11- } \\ & \text { O22 } \end{aligned}$ |  |
| 00 |  | 1.41 |  |  | 2.83 |  |  | 4.24 |  |  |  |  | 7.07 |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  | $\begin{aligned} & \mathrm{H} 12- \\ & \mathrm{H} 22 \\ & = \end{aligned}$ |  |  |  |  |  |  |
|  |  | $\begin{array}{\|l\|} \hline \mathrm{H} 12- \\ \mathrm{H} 12 \\ \hline \end{array}$ |  | $\begin{array}{\|l\|} \hline \mathrm{H} 11- \\ \mathrm{H} 12 \\ \hline \end{array}$ | $\begin{aligned} & \mathrm{H} 11- \\ & \mathrm{H} 11 \end{aligned}$ |  |  | $\begin{aligned} & - \\ & \hline \text { H11- } \\ & \text { H21 } \end{aligned}$ | $\begin{array}{\|l\|} \hline \text { H12- } \\ \text { H22' } \end{array}$ | $\begin{aligned} & \mathrm{H} 11- \\ & \mathrm{H} 21^{\prime} \\ & \hline \end{aligned}$ |  | $\begin{aligned} & \mathrm{H} 11- \\ & \mathrm{H} 22 \\ & \hline \end{aligned}$ |  |  |
| HH |  | 1.41 |  | 2.65 | 2.83 |  |  | 4.24 | 4.47 | 5.10 |  | 6.56 |  |  |

