ECCB'2003
Sept 27-30, 2003

$$V = \frac{1}{2} \Sigma k \Delta R^2$$

γ = force constant $\left[\frac{N}{m} = \frac{kg\ m}{m\ s^2} = \frac{kg}{s^2}\right]$

$B_i^{teor} = \sum_j C_{ij}^2 / k_j$ — autovalores (del cálculo del programa)

$\frac{B_i^{exp}}{B_i^{teor}} = \gamma^{-1} \Rightarrow B_i^{teor,\ reescalado} = B_i^{exp} \cdot B_i^{teor}\ \gamma^{-1}$

∴ obtengo los $B_i^{teor,\ reescalado}$ y con ellos calc. $\langle \Delta R_i^2 \rangle$

$$\langle R_i^2 \rangle = \frac{3}{8\pi^2} B_i^{teor,\ reescalado}$$

$$\Rightarrow \frac{\langle \Delta R_i^2 \rangle}{B_i^{teor}} = \frac{3 k_B T}{\gamma} = X = cte \quad (\text{para todo } i)$$

$X\ [\text{Å}^2]$