$\tilde{\nu}_i$ (AMBER) $\rightarrow k_i$

$$\lambda_i^{PCA}\,[\text{Å}^2] = \frac{108{,}879}{\tilde{\nu}_i\,(\text{AMBER})\,[\text{cm}^{-1}] \times 0{,}6}$$

k_BT [kcal/mol] = 0,593

Deducción:

$$k_i = \frac{k_BT}{\lambda_i^{PCA}} \qquad \nu_i = \sqrt{k_i}/2\pi$$

y ya que $\omega_i = \sqrt{k_i}$ y $\omega_i = 2\pi\nu_i$

$$\nu_i = \frac{1}{2\pi}\sqrt{\frac{k_BT\,[\text{kcal/mol}]}{\lambda_i^{PCA}\,[\text{Å}^2\,gr]}}$$

→ frecuencias de los mass weighted eigenvectors

$$1\ kJ = 1000\ kg\,\frac{m^2}{s^2}$$

$$1\ kcal = 4{,}184 \times 1000 \times 1000\,gr \times \frac{m^2}{s^2}$$

$$\nu_i = \frac{1}{2\pi}\frac{\sqrt{0{,}6}\times\sqrt{4{,}184\times 1000\,gr\times 1000}}{\sqrt{\lambda_i^{PCA}}\ \text{Å}\ \sqrt{gr}}\ \frac{m}{s}$$

$$= \frac{1}{2\pi}\frac{10^{10}\,\text{Å}}{s}\ \sqrt{0{,}6}\ \frac{\sqrt{gr}}{\text{Å}\sqrt{gr}} \times 2045{,}48$$