

Effect of temperature on enzyme activity.
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Enzyme reaction rate "constant" is a product of the rate constant leading to the product, k_2 , and the amount of active enzyme, E_{active} .

$$v = k_2 \cdot E_{\text{active}}$$

With enzyme deactivation, active enzyme decreases exponentially with time. Consequently, the enzyme reaction rate too decreases exponentially with time.

$$\frac{d}{dt} E_{\text{active}} = -k_d \cdot E_{\text{active}} \longrightarrow E_{\text{active}} = E_0 \cdot \exp(-k_d \cdot t) \longrightarrow v = k_2 \cdot E_0 \cdot \exp(-k_d \cdot t)$$

where the reaction rate "constants" k_2 and k_d depend on temperature in an Arrhenius fashion, with activation energies of E_a and E_d , or equivalently with activation temperatures of T_a and T_d , respectively.

$$k_2 = A \cdot \exp\left(-\frac{E_a}{R \cdot T}\right) \quad k_2 = A \cdot \exp\left(-\frac{T_a}{T}\right)$$

$$k_d = B \cdot \exp\left(-\frac{E_d}{R \cdot T}\right) \quad k_d = B \cdot \exp\left(-\frac{T_d}{T}\right)$$

Thus, reaction rate now depends on both temperature and time.

$$v(T, t) = A \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot \exp\left(-B \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t\right)$$

To find the temperature at which v is maximum, solve $dv/dT=0$. Here we mark "T" in the above equation and choose [Symbolic]Differentiate on Variable].

$$\frac{d}{dT} v(T, t) = A \cdot \frac{T_a}{T^2} \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot \exp\left(-B \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t\right) - A \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot B \cdot \frac{T_d}{T^2} \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t \cdot \exp\left(-B \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t\right)$$

We subsequently find $dv/dT=0$ with "Given-Find". Or, one can first mark T, then choose [Symbolic]Solve for Variable].

Given

$$dv/dT=0 \quad 0 = A \cdot \frac{T_a}{T^2} \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot \exp\left(-B \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t\right) - A \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot B \cdot \frac{T_d}{T^2} \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t \cdot \exp\left(-B \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t\right)$$

$$\text{Find}(T) \rightarrow \frac{-T_d}{\ln\left[\frac{T_a}{B \cdot (T_d \cdot t)}\right]}$$

Thus, the temperature at which v is maximum is:

$$T_{\text{max}} = \frac{-T_d}{\ln\left(\frac{T_a}{B \cdot T_d \cdot t}\right)}$$

Note that the temperature of maximum activity does not depend on the pre-exponential factor for k_2 nor E_0 , but it does depend on the pre-exponential factor for k_d and t , as well as the activation energies.

To find the maximum v , copy the RHS, mark T in the rate expression below, and choose [Symbolic]Substitute for Variable]:

$$v = A \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot \exp\left[-\left(B \cdot \exp\left(-\frac{T_d}{T}\right)\right) \cdot t\right]$$

Maximum v

$$v_{\max} = A \cdot \exp\left(\frac{T_a}{T_d} \cdot \ln\left(\frac{T_a}{B \cdot T_d \cdot t}\right)\right) \cdot E_0 \cdot \exp\left(\frac{-T_a}{T_d}\right)$$

Plot for specific parameter values (taken from Shuler & Kargi, Figure 3.15)

$$R := 0.0019872 \frac{\text{kcal}}{\text{mole} \cdot \text{K}}$$

$$E_a := 11 \frac{\text{kcal}}{\text{mole}} \quad A := 10^8 \text{ min}^{-1} \leftarrow \text{chosen to yield activity} \sim O(1)$$

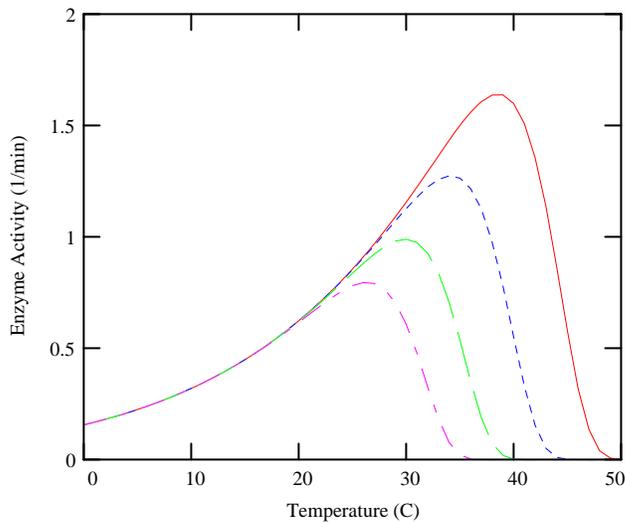
$$T_a := \frac{E_a}{R} \quad E_0 := 1$$

$$E_d := 70 \frac{\text{kcal}}{\text{mole}} \quad B := 10^{49} \text{ min}^{-1} \leftarrow \text{chosen to yield } T_{\max} \text{ around ambient.}$$

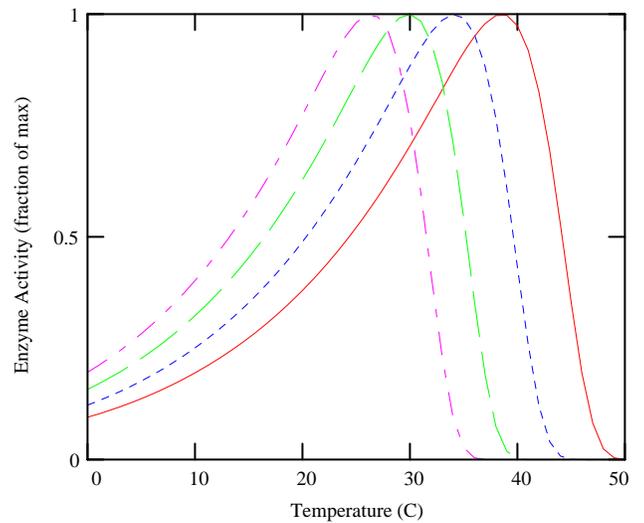
$$T_d := \frac{E_d}{R}$$

$$v(T, t) := A \cdot \exp\left(-\frac{T_a}{T}\right) \cdot E_0 \cdot \exp\left(-B \cdot \exp\left(-\frac{T_d}{T}\right) \cdot t\right) \quad v_{\max}(t) := A \cdot \exp\left(\frac{T_a}{T_d} \cdot \ln\left(\frac{T_a}{B \cdot T_d \cdot t}\right)\right) \cdot E_0 \cdot \exp\left(\frac{-T_a}{T_d}\right)$$

$$T := 273 .. 323$$



— 0.2 min
- - 1 min
— 5 min
- - 20 min



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- - 1 min
— 5 min
- - 20 min