

# Catalysis

Catalysis is thought to arise primarily from a lowering of the activation energy. Using the Arrhenius model calculate the difference in activation energy using only the data at 460 K provided below.

|                           |      |
|---------------------------|------|
| T (K)                     | 460  |
| Cat ( $M^{-1} s^{-1}$ )   | 130  |
| Uncat ( $M^{-1} s^{-1}$ ) | 0.25 |

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Solution: Given the data

|   |      |
|---|------|
| T (K)                                   | 460  |
| Cat ( $\text{M}^{-1} \text{s}^{-1}$ )   | 130  |
| Uncat ( $\text{M}^{-1} \text{s}^{-1}$ ) | 0.25 |

We can compare two rate constants with two different activation energies:

$$k_{cat} = A \exp \left\{ -\frac{E_{a,cat}}{RT} \right\}$$

and

$$k = A \exp \left\{ -\frac{E_a}{RT} \right\}$$

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The ratio of the two equations is:

$$\frac{k_{cat}}{k} = \exp \left\{ \frac{E_a - E_{a,cat}}{RT} \right\}$$

We solve for the difference in the activation energies to find:

$$E_a - E_{a,cat} = RT \ln \left( \frac{k_{cat}}{k} \right)$$

Inserting the numbers:

$$E_a - E_{a,cat} = (8.31)(460) \ln \left( \frac{130}{0.25} \right)$$

Therefore,

$$E_a - E_{a,cat} = 23,900 \text{ J/mol}$$

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In problem 1 we calculated the activation energies using the Arrhenius model. The difference between those values is:

$$E_{a,exp1} - E_{a,cat,exp1} = (70.5 - 44.9) \text{ kJ/mol}$$

$$E_{a,exp1} - E_{a,cat,exp1} = 25.6 \text{ kJ/mol}$$

Thus, the majority of the acceleration in rate is due to the lowering of the barrier. If the experimental error is 10% then the values obtained by the two considerations are within that range.