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Chemical Dynamics: Lecture 2 - Chemical Kinetics (Part 2)

We started the lecture with the continuation of chemical kinetics, picking up with second order reactions. For a generic reaction $A \rightarrow \text{Products}$, the rate law $R=k[A]^2$ was integrated (to make it into $y=mx +b$) form.

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(9) $k_2 k_2 = 2.2 + Q / Q R 2 (Q - Q R) 2 + V 2 (k B T) 2$

In an AI-TST calculation for an abstraction reaction, knowledge of the accuracy in predicted heats of formation can be used to assign an uncertainty to the Boltzmann factor in the barrier height.

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