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A satisfactory theory of these reactions was proposed by F. A. Lindemann in 1922. According to Lindemann, a unimolecular reaction $ A \longrightarrow P $ proceeds via the following mechanism: $ A + A \rightleftharpoons A^* +A $ Here the rate constants being $ k_f $ for forward reaction & $ k_b$ for backward reaction and

The Lindemann Theory of Unimolecular Reactions - Chemistry

The Journal of Physical Chemistry A 2007, 111 (19) , 3862-3867. DOI: 10.1021/jp0665675. J. Troe. Theory of Multichannel Thermal Unimolecular Reactions. 2. Application to the Thermal Dissociation of Formaldehyde. The Journal of Physical Chemistry A 2005, 109 (37) , 8320-8328. DOI: 10.1021/jp051027d.

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Theory of Thermal Unimolecular Reactions in the Fall-off ...
Collision Efficiency Parameter Influence on Pressure-Dependent Rate Constant Calculations Using the SS-QRRK Theory. The Journal of Physical Chemistry A 2020, 124 (31) , 6277-6286. ... Simplified Analysis and Representation of Multichannel Thermal Unimolecular Reactions. The Journal of Physical Chemistry A 2019, 123 (5) , 1007-1014.

Predictive possibilities of unimolecular rate theory | The ...
In chemical kinetics, the Lindemann mechanism is a schematic reaction mechanism for unimolecular reactions. Frederick Lindemann and J. A. Christiansen proposed the concept almost simultaneously in 1921, and Cyril Hinshelwood developed it to take into account the energy distributed among vibrational degrees of freedom for some reaction steps. It breaks down an apparently unimolecular reaction into two elementary steps, with a rate constant for each elementary step. The rate law and rate equation

Lindemann mechanism - Wikipedia
Transition States in Unimolecular Reactions, Theory of Unimolecular Reactions, 10.1016/B978-0-12-262350-9.50020-7, (344-393), (1973). Crossref Progress in Physical Organic Chemistry, Volume 9

Thermal Unimolecular Reactions - Willcott - 1972 ...
Until about 1921, chemists did not understand the role of collisions in unimolecular processes. It turns out that the mechanisms of such reactions are actually quite complicated, and that at very low pressures they do follow second-order kinetics. Such reactions are more properly described as pseudounimolecular. The cyclopropane isomerization described in Example 1 is typical of many decomposition reactions found to follow first-order kinetics, implying that the process is unimolecular.

6.1.6: The Collision Theory - Chemistry LibreTexts
d[A ∗] dt = k1[A][M](forward first step) − k − 1[A ∗][M](reverse first step) − k2[A ∗](forward second step) According to the steady-state approximation, d[A ∗] dt ≈ 0. Therefore the rate of production of A ∗ (first term in Equation 29.6.3) equals the rate of consumption (second and third terms in Equation 29.6.3):

29.6: The Lindemann Mechanism - Chemistry LibreTexts
unimolecular reactions in vapour phase: 1) LINDEMANN THEORY: According to this theory a unimolecular reaction A-> P proceeds via following mechanism: A* (P) Product. Where, A*=energized A molecule that has acquired sufficient energy to enable it to isomerizes or decomposed i.e., the vibration.

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The Rice–Ramsperger–Kassel–Marcus theory is a theory of chemical reactivity. It was developed by Rice and Ramsperger in 1927 and Kassel in 1928 and generalized in 1952 by Marcus who took the transition state theory developed by Eyring in 1935 into account. These methods enable the computation of simple estimates of the unimolecular reaction rates from a few characteristics of the potential energy surface.

RRKM theory - Wikipedia
Unimolecular Reactions of Peroxy Radicals in Atmospheric Chemistry and Combustion. ... MESMER: An Open-Source Master Equation Solver for Multi-Energy Well Reactions, The Journal of Physical Chemistry A, 10.1021/jp3051033, 116, 38, (9545-9560), (2012 ... Journal of Chemical Theory and Computation, 10.1021/ct200011e, 7, 5, (1244-1252), (2011 ...

Unimolecular Reactions of Peroxy ... - Chemistry Europe
The quantum tunneling contribution to the reaction rate constants is calculated using the semiclassical transition state theory (SCTST) developed by Miller and co-workers. 26–31 The SCTST calculates the overall quantum tunneling probability by summing over a series of TS vibrational configuration-dependent tunneling probabilities.

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