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Introducing the Effective Mass of Activated Complex and the Discussion on the Wave Function of this Instanton

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Evaluation category: Contribution to knowledge

Description of the result:

The monograph: Introducing the Effective Mass of Activated Complex and the Discussion on the Wave Function of this Instanton, whose authors are Petr Ptáček, Tomáš Opravil and František Šoukal, presents a newly developed method for studying the kinetics of processes in which the phase interface moves, or the spatial arrangement of phases changes, which occurs in the majority of industrially important processes. This newly developed method combines universality, an effective way to determine the result and an innovative approach that allows for a quick and comprehensive evaluation of the course of the process depending on the conditions that affect it.

The mentioned comprehensive evaluation means in particular the evaluation of the activation energy (E_a), the frequency factor (A) and the mechanism (n) of the ongoing process:

(1)
$$E_a = \bar{\boldsymbol{v}}_g^2 T_r^2 M^\# = \gamma \frac{p}{\rho_0}\left(\frac{T_{m,\Theta 1}}{298.15}\right)^2 M^\# = const.'' \, T_{m,\Theta 1}^2 M^\#$$

Where:

Composition of the gas phase		$\boldsymbol{\rho_{0°C}}$	$\boldsymbol{\gamma = c_p/c_v}$	$\boldsymbol{\bar{v}_{(g)}}$	$\boldsymbol{const.'''}$	$\boldsymbol{const.''}$
		[kg·m^{-3}]	---	[m·s^{-1}]	[m·K^{-1}·s^{-1}]	[m^2·K^{-2}·s^{-2}]
Air		1.2959	1.404	331.3	1.111	1.235
Nitrogen	N_2	1.2510	1.404	337.2	1.131	1.279
Oxygen	O_2	1.1429	1.400	315.1	1.057	1.117
Carbo dioxide	CO_2	1.9770	1.288	256.9	0.862	0.743
Argon	Ar	1.7838	1.668	307.8	1.032	1.066

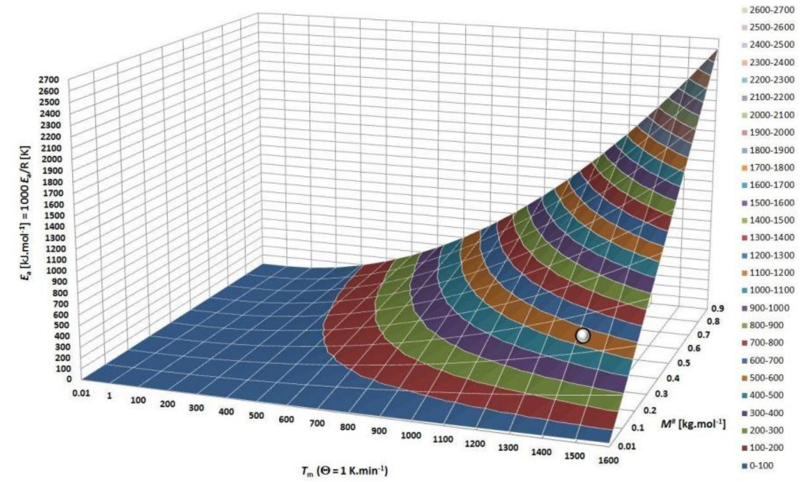
And $M^\#$ denotes the effective mass of the activated state:

(2)
$$M^\# = \frac{R\left(ln\left[\frac{T_{m,\Theta e}^2}{T_{m,\Theta 1}^2}\right] - 1\right)}{const.''\left(\frac{T_{m,\Theta 1}^2}{T_{m,\Theta e}} - T_{m,\Theta 1}\right)} \cong \frac{\mathrm{K}_T}{\Delta T_m}$$

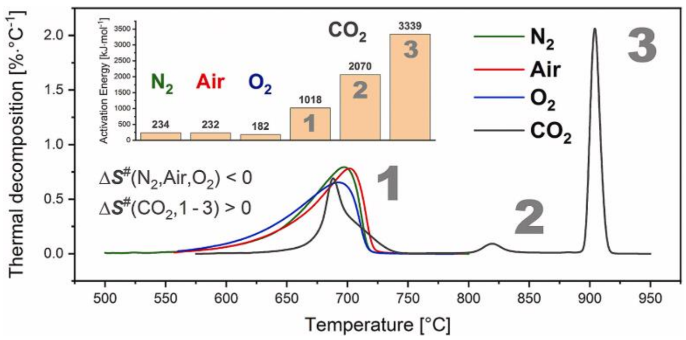
Where the constant K_T has the same physical dimension as the ebullioscopic constant, i.e. $K \cdot kg \cdot mol^{-1}$.

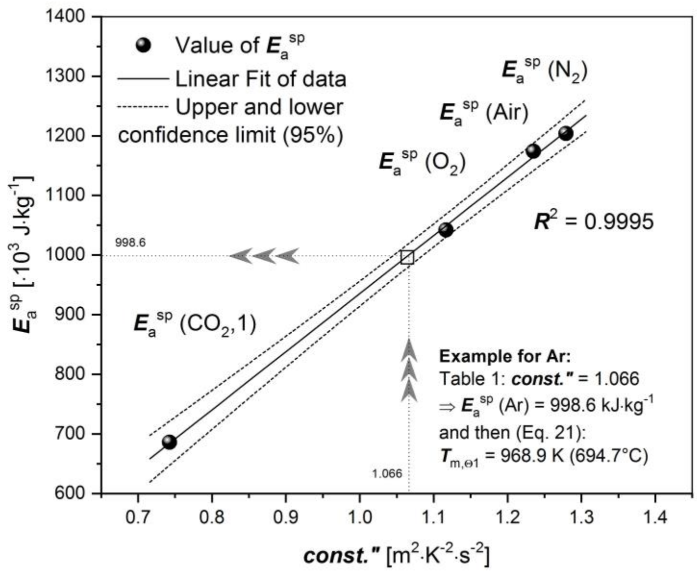
(3)
$$A = \frac{2.5\ exp\left(\frac{E_a}{RT_{m,\Theta 1}}\right)}{60\ w_{1/2,\Theta 1}} = \frac{1}{24}\frac{exp\left(\frac{T'}{T_{m,\Theta 1}}\right)}{w_{1/2,\Theta 1}}$$

(4) $$n = \frac{2.5\ RT_{m,\Theta 1}^2}{w_{1/2,\Theta 1}E_a} \approx \frac{2.5\ |\Delta T_m|}{w_{1/2,\Theta 1}}$$



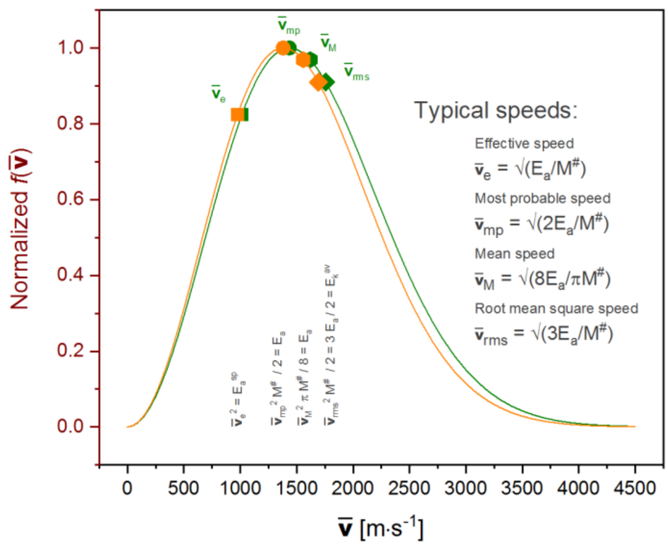
The practical use of these formulas then requires only two experiments performed with a heating rate of 1 and e = 2.717… (Euler's number) $°C \cdot min^{-1}$. In this regard, it is necessary to emphasize that scientific papers dealing with kinetics mostly publish information only on the activation energy. However, data on the frequency factor and the mechanism are necessary to calculate the course of the process and its modeling under the given conditions. It is not even possible to perform such calculations without them. The approach enabling the rapid evaluation of complex kinetic data thus becomes a fundamental advantage of this method.



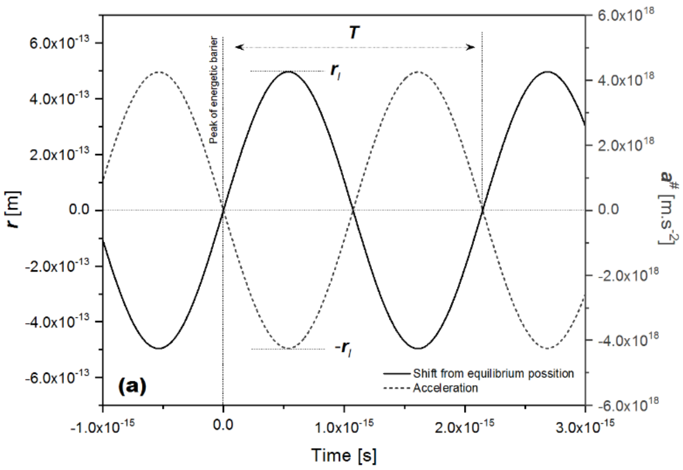


It is also unique in that it is the only one of all known procedures that also includes the influence of the environment in which the process takes place. So, for example, the way in which the composition of the gas above the solid will affect the activation energy of the ongoing process. In this regard, a really interesting finding is the fact that the increasing content of carbon dioxide in the atmosphere generally increases the activation energy of processes, even those in which CO_2 is not directly involved in the reaction.

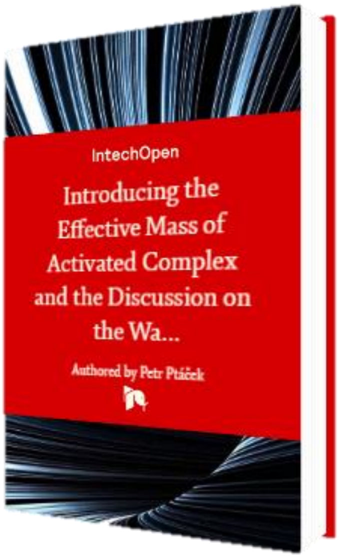
Despite this, however, it is an approach that is faster and more universal than the kinetic study methods used so far. Another benefit of the mentioned approach is that it naturally allows one to apply the Maxwell-Boltzmann distribution of energies to the activated system. One of the scientifically significant consequences of such an approach is that during a chemical reaction, the average energy of an activated set of molecules is one and a half times higher than the activation energy, i.e. the energy required to overcome the energy barrier.

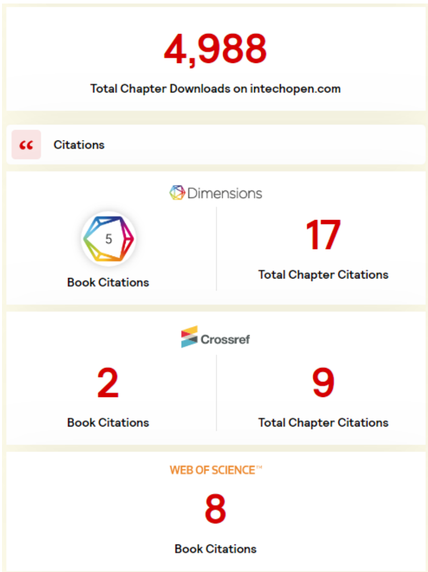


Another is that it introduces the first experimental procedure by which it is possible to determine the effective mass of the activated complex ($M^{\#}$, equation 4). Its momentum can then be calculated from this information. Together with the activation energy, this represents a pair of quantum numbers that characterize the activated molecule. Ultimately, the wave function of the activated complex can thus be derived.



The monograph comprehensively introduces the possibilities of using this method, the beginning of which was the findings published in a foreign scientific journal with a high IF in the field (impact factor 5.532) - Ceramics International: The formation of feldspar strontian ($SrAl_2Si_2O_8$) via ceramic route: Reaction mechanism, kinetics and thermodynamics of the process. It also became the basis for ever-developing research, the latest published output of which is an article in the journal Solid State Sciences (IF 3.752): Thermal decomposition of ferroan dolomite: A comparative study in nitrogen, carbon dioxide, air and oxygen. The top world level of the book can be proven by its response in the professional community. Since its publication in 2018, it has been downloaded almost 5000 times and cited 17 times, of which 8 times on Web of Science.





Počet stažení za posledních 6 měsíců, dle krajin:

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