



The chemical equilibrium on the test bench Why clouds do not fall from the sky

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1. Introduction

The protolysis of acetic acid in water or the esterification of acetic acid and ethanol are considered key experiments in high school chemistry lessons -- experiments that occur spontaneously and serve the introduction or application of the law of mass action. If one takes the trouble and calculates the change of the standard Gibbs enthalpy ΔG° for these processes one arrives at the prediction, both processes are endergonic and should not be spontaneous. In this paper, a sub--aspect of a PhD project on "From Chemical Potential to Chemical Equilibrium" is presented, which uses this contradiction as an opportunity to point the way to the law of mass action without kinetic derivation. If we link the metabolic rate (x) and energy turnover of a chemical reaction and consider this as a process, the Gibbs enthalpy $G(x)$ always has a minimum in equilibrium reactions. Using spreadsheets, Gibbs enthalpy can be represented as $G(x)$ for ester formation, organic acid protonation, butane isomerization, and other teaching--related processes.

With regard to the experimental realization of processes, the maximum principle of entropy of intuition is often more conducive than the minimum principle of energy (Falk 1984). The possibility of giving the rubber elasticity the Gibbs-Helmholtz equation is discussed in an experiment (heating an overstretched rubber band).

In addition, it is shown how the description of state changes using the Gibbs--Helmholtz equation allows access to current concepts such as the entropy force. A look at the core curricula Chemistry of the Federal States of North Rhine-- Westphalia and Lower Saxony offers initial approaches to evaluation.

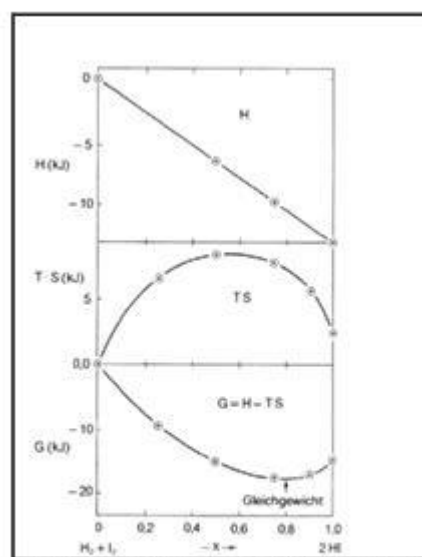


Abb. 1 Funktion Enthalpie (H), Entropie (TS) und Gibbs-Funktion (G) für die Jodwasserstoffreaktion (Pimentell, 1978, S. 188)

2. Events

The chemical equilibrium in Secondary Level II chemistry lessons is constantly under scrutiny (Tittel, Kremer 2017). In addition to the qualitative description of the chemical equilibrium as a state of simultaneous presence of educts and products, the kinetic interpretation assumes a dynamic equilibrium with equally high forward and backward reaction rates. The reaction order for the formulation of the reaction rate is derived from the reaction equation, although the reaction order of a chemical reaction can not usually be derived from the reaction equation (Atkins 1996, p.818). A Chemistry book of secondary education (Asselborn 2009, p. 107) describes the problem as follows "An essential pillar for the establishment of the law of mass effects was an assumption that is currently inadmissible: it was assumed that the equation of speed of a reaction is always direct derived from the reaction equation ". This assumption was based on

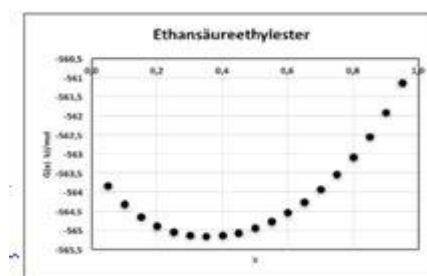


Abb. 2 Funktionale Verlauf $G(x)$ einer endergonischen Reaktion (eigene Illustration)

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Max Bodenstein's work on the formation and decomposition of hydrogen iodide gas (Bodenstein 1894). A first approach to represent the process of adjusting a chemical equilibrium is found in Pimentell (Fig. 1).

3. Process

Ludwig Boltzmann is the first to describe the entropy of a system as a state variable S . To do this, he links the entropy with the thermodynamic probability W .

The thermodynamic probability W indicates the number of distribution possibilities (microstates) that can be used for a system with a constant overall state (macrostate). gives. The Gibbs--Helmholtz equation, in the form of $\Delta G = \Delta H - T\Delta S$ applied to the formation of ethyl ethanoate, yields the result $\Delta G > 0$ and leads to the prediction that this reaction is endergonic and may be due to the sign of the change Gibbs enthalpy does not happen spontaneously. This contradicts the observation.

An important aspect of the PhD project is the modeling of the formation of hydrogen iodide adjustment of the chemical equilibrium from the point of view of substance dynamics (Fig. 2). For this purpose, the possibility of using an approximation function (Stirling formula) to describe the entropy in the form $S(x)$ is used (Salm 1997, p.51). For a of the form $A + B \rightleftharpoons 2C$ (Figure 3) then the input function for the spreadsheet is:

$$G(x) = (1-x)G^{\circ}A + (1-x)G^{\circ}B + 2xG^{\circ}C + 2xRT \ln x + 2(1-x)RT \ln(1-x).$$

4. Performance

The inclusion of the statistical interpretation of the entropy $S(x)$ and the formulation of the Gibbs enthalpy G as a functional curve $G(x)$ allows the prediction of chemical equilibria, regardless of whether the complete reaction is classified as exergonic or endergonic.

Nearly all lesson--relevant donor--acceptor equilibria such as acid--base or red--ox can be detected. The efficiency of this process is also illustrated by the example of autoprotolysis of water (Figure 4).

The minimum of the functional course of $G(x)$ is $x = 10^{-7}$ ($\text{CH}_3\text{O} + = 10^{-7} \text{ mol/L}$).

Furthermore, the method offers interpretation aids in the exploration of material properties such as e.g. the rubber elasticity or absorbency of hydrogels (Figure 5). The quotient dG/dl turns out to be a known quantity, namely that of a force. This entropic power as restoring force is explained by the desire for maximum entropy and is recognizable by the minimum of Gibbs enthalpy.

Concepts for entropic gravity are currently being discussed (Verlinde 2010). Scattering of particles due to Brownian motion causes delays in entropy forces. Thus, due to the desire for maximum

$$F = \frac{dG}{dl} = \frac{d(H - TS)}{dl} = \frac{dH}{dl} - \frac{TdS}{dl}$$

entropy, a cloud experiences a force opposite to the weight FG and does not fall from the sky (Figure 6).

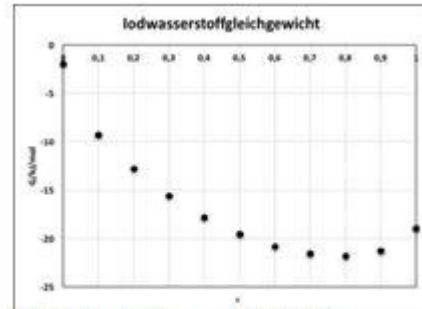


Abb.3 Functional curve $G(x)$ for the formation of hydrogen iodide (Own Illustration)

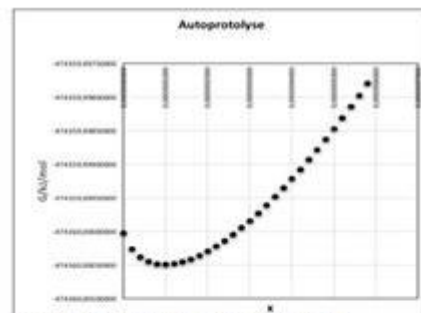


Abb. 4 Functional course $G(x)$ with minimum at $x = 0.0000001$ (own illustration)

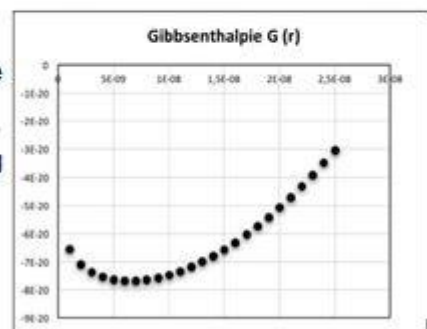


Abb. 5 Functional course of Gibbsenthalpy $G(r)$ as a function of the end distance r of a macromolecule (own illustration)



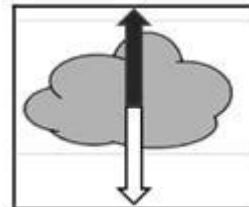
5. Conclusion and outlook

The teaching pathway Material Dynamics "Chemical equilibrium" $G(r)$ as a function of the end to end distance r of a macromolecule (own can be considered as a mediator between university expertise and illustration) the required professional knowledge of a chemistry teacher.

The departure from the description of the state by means of the Gibbs-Helmholtz equation to the description of the process of adjusting the chemical equilibrium makes further balancing possible.

The functional course of the Gibbs enthalpy $G(x)$ supplies the position of the equilibrium. The length-related rate of change dG/dl describes a force F , which has a temperature dependence in contrast to the Newtonian idea.

The substance-related rate of change dG/dn provides the chemical potential μ , which in turn is temperature-dependent. As a result, this quantity μ also differs from the physical potential. A decision for the static interpretation of entropy S in chemistry lessons from the beginning (without resorting to circular processes of thermodynamics) opens up possibilities of current contextualization. The efficiency derived from the Gibbs-Helmholtz equation offers occasions of evaluation and interpretation. High entropy change processes ΔS (complete phase change oxidation) differ significantly in the efficiency of low entropy change processes ΔS (electron transfer reactions in primary and secondary elements).



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