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Write an expression for the equilibrium constant of each chemical equation

For experimental methods and computational details, see Determination of balance constants. The constant balance of a chemical reaction is the value of the reaction quotient to the chemical balance, a state approached by a dynamic chemical system after sufficient time has passed where its composition has no measurable tendency towards a further change. For a given series of reaction conditions, the balance constant is independent of the initial analytical concentrations of reactionary and product species in the mixture. Thus, given the initial composition of a system, the known balance constant values can be used to determine the composition of the system in balance. However, reaction parameters such as temperature, solvent and ion resistance can affect the value of balance constant. A knowledge of balance constants is essential for understanding many chemical systems, as well as biochemical processes such as transporting oxygen from hemoglobin in blood and omeostasis acid-base in the human body. Stability constants, formation constants, binding constants, association constants and dissociation constants are all kinds of balance constants. Definitions and basic properties For a reversible reaction system described by the general chemical equation $\alpha A + \beta B + \text{appearance} \rightleftharpoons \rho R + \sigma S + \sigma$ $\displaystyle \alpha \mathrm{A} +\beta \mathrm{B} +\cdots \rightleftharpoons \rho \mathrm{R} + Qt$ when reactions forward and reverse occur at the same pace. To the chemical balance, the chemical composition of the mixture does not change with time and change of free energy Gibbs ΔG $\displaystyle \Delta G$ for reaction is zero. If the composition of a mixture in balance is changed by addition of some reagent, a new balance position will bel've given enough time. A balance constant is linked to the composition of the mixture in balance of [1][2] K di = {R } ρ {S } σ . . . {A } α {B } β . . = [R] ρ [S] σ . . . . α [B] β . . . . . . × , $\displaystyle K^{\ominus}$ Translation: # ♪ ♪ == sync, corrected by elderman == @elder_man If it is assumed that the quotient of coefficients of activity, , is constant on a range of experimental conditions, such as pH, then a balance constant can be derived as a quotient of concentrations. K = K . / I = R ρ σ σ . . . . A balance constant is linked to the standard free energy change of Gibbs reaction Δ G . $\displaystyle \Delta G^{\ominus}$ by Δ G . = − R T ln K . , $\displaystyle \Delta G^{\ominus}=-RT\ln K^{\ominus}$ where R is the constant of universal gas, T is the absolute temperature (in kelvins), and ln is a logaritmo This expression implies that K . $\displaystyle K^{\ominus}$ must be a pure number and cannot have a dimension, since logarithms can only be taken of pure numbers. K c $\displaystyle K_{c}$ must also be a pure number. On the other hand, the reaction quotient to the balance [R] ρ [S] σ . . . . ♪ Translation: }...}{\mathrm {A} }^{\alpha }\mathrm {B} }^{\beta }...}{eq}} has the size of the concentration raised to a certain power (see #Dimensionality, below). Such reaction quotients are often indicated, in biochemical literature, as balance constants. For a mixture of gas balance, a balance constant can be defined in terms of partial or fleeting pressure. A balance constant is linked to the speed constants forward and backward, kf and kr of the reactions involved in achieving balance: K : = k f k r . $\displaystyle K^{\ominus}$ Translation: {k _{\text{f}}}{k _{\text{r}}}}} Types of constant balance constants of cumulative and passive formation A cumulative or overall constant, given the β symbol, is the constant for the formation of a reagent complex. For example, the cumulative constant for the formation of ML2 is given by M + 2 L⇌ ML2; [ML2] = β12[M][L]2 The constant stepwise, K, for the formation of the same complex from ML and L is given by ML + L⇌gene ML2; [ML2] = K[ML][L] = Kβ11[M][L]2 It follows that β12 = Kβ11 A cumulative constant can always be expressed as the product of constant stepwise. There is no notation apart from the β symbol, although a symbol like KLML is sometimes found in literature. It is better to always define every constant stability by referring to an expression of balance. A particular use of a constant step-by-step is in the determination of constant values of stability outside the normal range for a given method. For example, EDTA complexes of many metals are outside the range for the potentiometric method. Stability constants for those complexes were determined by competition with a weaker binder. ML + L′ == == == == == == == == == == == == == == == == == == ?? ? ?? ?? ?? ?? ?? ?? ?? ?? == == ? ? ? == =translation: {\ \mathrm {ml} }=K\beta {\ \mathrm {ml} }} the training constant of [Pd(CN)4]2− was determined by the competition method. associations and constant dissociations in organic and biochemistry is customary to oate pka values for balances of acid dissociation. k a = − log k d i s = log (1 k d i s) $\displaystyle \mathrm {p} K_{\mathrm {a} -\!=}\log K_{\mathrm {diss}} \!=\log \left({\frac {1}{K_{\mathrm {diss}} right},$ where the log indicates a logaritmo at the base for the bases, the association of constant base, pkb is used. for any acid or base data the two constants are connected by pka + pkb = pkw, so pka can always be used in calculations. On the other hand, stability constants for metallic complexes, and binding constants for guest-guest complexes are generally expressed as association constants. when considering the balances as m + hl ⇌ ml + h is customary constant oare of association both for ml and for hl. moreover, in generalized computer programs that deal with balance constants in the general practice of oare cumulative constants rather than constant step-by-step and to omit ionic burdens from balance expressions. For example, if nta, nitrilotriacetic acid, N(CH2CO2H)3 is designated as h3l and complex form ml and mhl with a metallic ion m, the following expressions would apply for constant dissociation. ;) — − ; ; ; ; ; ; ; ; ; ((( )) ; ; ; ; ; ; ; ; ; ; ;) ;)) {H2L {HL}+H}}; &{\ce {p}}K_{2}=\log \left({\frac {[{\ce {HL}}]{[{\ce {H}}]{\ce {H}}}{\ce {H=}{\ce}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\c}{\V } (a) the Commission's decision on the application of the provisions of Article 2(1) of Regulation (EEC) No 1408/71. Note how the subscribers define the stoichymetry of the balance product. Microcosters When two or more sites in an asymmetric molecule can be involved in a balance reaction there are more than one possible balance constant. For example, the L-DOPA molecule has two non-equivalent hydroxylic groups that can be deprotonate. Denoting L-DOPA as LH2, the following diagram shows all species that can be formed (X = CH2CH(NH2)CO2H). The concentration of the species LH is equal to the sum of the concentrations of the two microspecies with thechemical formula, labeled L1H and L2H. The constant K2 is for a reaction with these two micro-species as products, so that [LH] = [L1H] + [L2H] appears in the numberer, and follows that this macro-constant is equal to the sum of the two micro-constants for the reactions of the components. K2 = k21 + k22 However, the constant K1 is for a reaction with these two microspecies as reagents, and [LH] = [L1H] + [L2H] in the denominator, so that in this case[3] 1/K1 =1/k11 + 1/k12, and then K1 =k11 k12 / (k11 + k12.) Thus, in this example there are four micro-constants whose values are subject to two constraints; consequently, only the two macro-constant values, for K1 and K2 can be derived from experimental data. Micro-constant values can, in principle, be determined using a spectroscopic technique, such as infrared spectroscopy, where each microspecies gives a different signal. The methods that have been used to estimate micro-consistent values include Chemistry: blocking one of the sites, for example for the methylation of a hydroxyl group, followed by the determination of the relative molecule's equilibrium constant, from which the micro-consistent value for the parent molecule can be estimated. Mathematics: application of numerical procedures to NMR 13C[4][5] Although the value of a micro-constant cannot be determined by experimental data, the occupation of the site, which is proportional to the micro-constant value can be very important for biological activity. Therefore, various methods have been developed to estimate micro-costant values. For example, the isomerization constant for L-DOPA has been estimated to have a value of 0.9, so the L1H and L2H microspecies have concentrations almost equal to all pH values. In the approximation of the ideal behaviour, activity is replaced byThe pH is measured by means of a glass electrode, a mixed mixtureconstant, may result. HL⁻ L + H; p K = − log (L L { H } { H L } $\displaystyle \mathrm {p} K=\log \left({\frac {[\mathrm {L} {\mathrm {H} [{\mathrm {HL}\right}$ Everything depends on the fact that the electrode is calibrated in reference to known activity solutions or known concentration. In the latter case the balance constant would be a concentration quotient. If the electrode is calibrated in terms of known hydrogen ion concentrations it would be better to write p[H] rather than pH, but this suggestion is not generally adopted. hydrolysis constants In aqueous solution the concentration of hydroxide is linked to the concentration of hydrogen ion of K W = [H] [OH] $\displaystyle {\ce {\mathit Translation: K}}_{W}[H]^{-1 The first step in metal hydrolysis[6] can be expressed in two different ways {M(H) 2 O − − ' M (OH) + H; [M (OH)] = β [[M] − − − − −] M (OH) ; [M (O=) H] Hydrolysis constants are usually reported in the β* form and therefore often have values much less than 1. For example, if the K = 4 and the KW = −14, log β* = 4 + (−14) = −10 so that β* = 10−10. In general, when the hydrolysis product contains n hydroxide ion groups β* = log K + n log KW Conditional constants, also known as apparent constants, are concentration quotients that are not true balance constants, but can be derived from them. [7] A very common instance is where the pH is fixed at a particular value. For example, in the case of iron (III)with EDTA, a conditional constant could be defined by K c or n d = [Total Fe bound to EDTA] [Total Fe not bound to EDTA] × [Total EDTA not bound to Fe] $\displaystyle K_{\mathrm {cond} \# E' problema \# EDTA}]}]{[{\mbox{Total Fe not bound to EDTA}]}time]\mboxTotal Fe This conditional constant varies with pH. It has a maximum pH. This is the pH in which the binder seizes the metal more effectively. In biochemistry, balance constants are often measured at fixed pH through a buffer solution. These constants are, by definition, conditional and different values can be obtained when using different buffers. balancing the gas phase For balances in a gas phase, escapecity, f, is used in place of activity. However, evacuation has the size of the pressure, so it must be divided by a standard pressure, usually 1 bar, to produce a quantity without size, f/po. A constant balance is expressed in terms of quantity without size. For example, for the balance 2NO2⇌ N2O4, f N 2 O 4 p ' = K (f N O 2 p ') 2 $\displaystyle {\frac f_{\mathrm N_{2}O_{4} }p^{\ominus}=K\left({\frac f_{\mathrm NO_{2} } }p^{\ominus}\right}^{2^{2^{2^{2 Escapement is linked to partial pressure, p, by a non-dimensional evacuation coefficient φ: f = φp. Thus, for example, K = φ N 2 O 4 p N 2 O 4 / p φ (φ N O 2 p N O 2 / p)) 2 $\displaystyle Translation: # N_{2}O_{4} }p_{\mathrm N_{2}O_{4/}p^{\ominus}\phi {\ \mathrm N_{2} } } } } } } } } } } } } } φp_{\math_{\math_{\mathrm Usually the standard pressure is omitted by such expressions. Expressions for balance constants in the gas phase then resemble the expression for balance solution with escaping coefficient instead of the coefficient of activity and partial pressure instead of the concentration. K = φ N 2 O 4 p N 2 O 4 (φ N O 2 p N O 2 2) $\displaystyle K={\frac {\phi {\ \mathrm N_{2}O_{4 }p_{\mathrm {NO_{2}} }p_{\mathrm {NO_{2}} }\right}^{2}}}} The thermodynamic base for constant expressions of balance The thermodynamic balance is characterized by free energy for the whole system (closed) being a minimum. For constant temperature and pressure systems, Gibbs free energy is minimal. [8] The slope of energy without reaction compared to the co-ordinate reaction, ξ, is zero when free energy is at its minimum value. (∂ G ∂ ξ) T , P = 0 $\displaystyle \left({\frac {\partial G}{\partial \xi }}\right)_{T,P}=0$ Free energy change, δGr, can be expressed as a weighted sum of potential chemicals, the free partial molar energies of the balanced species. The potential, μi, of the ith species in a chemical reaction is the partial derivative of free energy compared to the number of molecules of that species, Ni μ i = (∂ G ∂ N i) T , P $\displaystyle \mu _{i}=\left({\frac {\partial G}{\partial N_{i}}}\right)_{T,P}$ A general chemical balance can be written as j n j r and a c t a n t j⁻‾ k r o d u c t k $\displaystyle \sum _{j}n {j}\mathrm - Yes. _{j}\rightleftharpoons \sum _{k}m _{k}\mathrm {Product} _{k}$ where nj are the stoichiometric coefficients of the reactives in the balance equation, and mj are the coefficients of the products. A equilibria | k μ k = Σ Σ Σ display reported in the β* form and therefore often have values much less than 1. For example, if the K = 4 and the KW = −14, log β* = 4 + (−14) = −10 so that β* = 10−10. In general, when the hydrolysis product contains n hydroxide ion groups β* = log K + n log KW Conditional constants, also known as apparent constants, are concentration quotients that species, R is the constant of the gas and T is the temperature. Set the sum for reactives j to be equal to the sum for products, k, so that δGr(Eq) = 0 sign j n j (μ j + + R T ln a j) = sign k m k (μ k + + R T ln φ a k) $\displaystyle \sum _{j}n_{j}(\mu _{j}^{\mu _{j}^{\mu _{j}}^{\ominus +}RT\ln a _{k}) Reorder the terms, | k m k μ k o − D P_j μ j − − R T (Σ k ln)} j a k m k − Đ ln }} j a k m k − Đ Δ G = − R T ln K . {\displaystyle \Delta G^{\ominus} Translation: This concerns the normal Gibbs free energy change, ΔGo to a balance constant, K, the reaction quotient of the values of activity to balance. ; display Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ display display display display display display display Σ Σ Σ Σ Σ Σ Σ display Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ Σ K={\frac {\prod k}{a_{k}}^{m_{k}}}{\prod a_{j}}^{n_{j}}}\equiv # Translation: Translation: # Mathrm # (B) }... Equivalence of thermodynamic and kinetic expressions for balance constants In balance the rate of reaction forward is equal to the reaction rate backwards. A simple reaction, such as the hydrolysis of the AB + H 2 O − − ' AH + B (OH) $\displaystyle {\AB + H2O