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Stability constants and thermodynamic properties of complexation of Ibuprofen with Zr^{4+}PH metrically

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Abstract: pHmetric studies of binary complex of $Zn^{4+}$with ibuprofen has been carried out in ethanol at three temperatures (25 ±0.1, 30 ±0.1 and 35± 0.1^0 C) and at an ionic strength of 0.1 mol L^{-1} (KNO_3). The thermodynamic parameters ΔG, ΔH and ΔS are calculated by known equation. pHmetric measurement of hydrogen ion concentration may be employed when the degree of complex formation is sensitive to the hydrogen ion concentration thus the degree of complex formation undergoes increase/ decrease with change in pH.. The method of Calvin and Bjerrum as adopted by Irving and Rossotti has been employed to determine log K1 values. The thermodynamic parameters ΔG, ΔH and ΔS are calculated.
Keywords: pH metry, Stability constant, Thermodynamic parameters, Free energy, Enthalpy, Entropy.

Introduction:

Ibuprofen is used primarily for fever Ibuprofen, from isobutylphenylpropanoic acid, is a nonsteroidal anti-inflammatory drug (NSAID) used for treating pain, fever, and inflammation[1] fever (including postimmunisation fever), mild-to-moderate pain (including pain relief after surgery), painful menstruation, osteoarthritis, dental pain, headaches and pain from kidney stones. It is used for inflammatory diseases such as juvenileidiopathic arthritis and rheumatoidarthritis.[2][3] .It is also used for pericarditis and patent ductusarteriosus[4].

The pKa values of ligands and stability constants of the complexes with some hydroxamic acids a comparative study of three different potentiometric methods was reported by Senthilnithy [5]. The data obtained by pH-metric method were analyzed by three standard methods namely, Bjerrum's method, Irving and Rossotti method, and Sarkar and Kruck method. Aectohydroxamic acid, $CH_3CONHOH$, forms highly stable complexes with vanadium (V) and vanadium (IV) in 1: 1, 1: 2 and 1 : 3 mole ratios [6]. The stability of these complexes can be determined in terms of thermodynamic parameters; ΔG, ΔH and ΔS . The preliminary data, obtained through pH titration at various temperatures, was processed. Another study on the stability constant of the transition metal complexes with some medicinally important compounds was reported by Chaudhari [7]. The formation of bioligand complexes of some medicinal drugs with Co (II), Ni (II) and Cu (II) ions were investigated. The formation const. of Ranitidine Hydrochloride and 6-methoxy naphthaldehyde has been carried out pH metrically in aq. soln. at 30°C, at 0.1 M fixed ionic strength [7]. The method of Calvin and Bjerrum [8,9] as adopted by Irving and Rossotti [10] has been employed to determine log K value

Material and methods:

The titration were carried out in a100 ml Pyrex glass beaker kept in a water bath maintain at constant temperature Chemicals and ligand used were of analytical grade. Ligand solutions were prepared in ethanol. Metal salt solutions were prepared by dissolving the corresponding metal salt in twice distilled deionized water and standardized by standard volumetric methods. The free hydrogen ion concentrations were measured with a combined glass electrode attached to digital pH meter model-361; the accuracy of pH meter was 0.01 at three temperatures (25 ± 0.1, 30 ± 0.1 and 35 ± 0.1° C) and at an ionic strength of 0.1 mol L^{-1} (KNO_3). The pH meter was calibrated with suitable buffers before use.

Result and discussion :

Calvin – BjerrumTitration :

The experimental procedure involved pHmetric titration of,
Free acid (0.01M) titration,
Free acid (0.01 M) and ligand (0.05M) titration.
Free acid (0.01M), ligand (0.05M) and metal ion (0.01M) against std. NaOH solution.

The ionic strength of all solutions were maintain constant (0.1M) by adding appropriate quantity of 1M KNO_3solution.

The titration were carried out in a100 ml Pyrex glass beaker kept in a water bath maintain at constant temperature (25,30and 35 ^{0}C) nitrogen gas was purged for chemically inert atmosphere. The readings were recorded for each addition of 0.1ml. The graphs of volume of alkali added against pH were plotted.

The titration curve of the acid and the ligand deviates at about pH 3.0 and then increase up to pH 12.0. The deviation between acid curve from ligand curve for the systems showed the dissociation of H^+ from-COOH groups of the ligands.

Proton – ligand formation Number (n^-A):

Proton – ligand formation number (n A) were calculated by Irving and Rossotti expression.

$nA = \gamma - (E^0 + N)(V_2 + V_1) / (V^0 + V_1) T^0_L$
Where, V^0 = Initial volume of solution (50 ml)
N = Normality of sodium hydroxide
T^0_L = Concentration of ligand in 50 ml solution
E^0 = Initial concentration of free acid (HNO_3)
γ = Number of dissociable proton from ligand
V_1 and V_2 – Volume of alkali consumed by acid and ligand on same pH

Metal- ligand formation number (n):

The deviation of (A + L +M) curve from (A +L) started at about pH 3.5, It indicate the commencement of complex formation .

Metal – Ligand formation number (n) was calculated by following expression.
$n = (E^0 + N)(V_3 - V_2) / (V^0 + V_2)(T^0_M) \times nA$
V^0 = Initial volume of solution (50 ml)
N = Normality of sodium hydroxide
T^0_M = Concentration of the metal ions
nA = Proton – ligand formation number
E^0 = Initial concentration of free acid (HNO_3)

Where, V_2 and V_3 – volume of NaOH consumed by ligand and metal ions at same pH.

Metal – Ligand Formation curves:

Formation Curves were plotted between n and p^H .The metal-ligand stability constants were determination by half integral method

Half Integral Method:-The metal- ligand stability constants (log, k_1 values) are calculated from formation curves. The values of n = 0.5 which corresponds to value of The valuesof Pk.The values of metal – ligand stability constants i.e. log k for all the systems were presented in tables.

Table: Stability constants and thermodynamic parameters of $Zr^{4+}$with Ibuprofen

System	**Temperature (^{0}C)**	**pKa**	**logK**	**-Δ H (KJmol^{-1}) At 30^{0}C**	**-Δ G (KJmol^{-1})**	**-Δ S (KJmol^{-1}deg^{-1}) At 30^{0}C**
Zr(IV)Ibuprofen	25	5.7446	7.265	5.50	41.452	0.12
	30	5.7385	7.185		41.683	
	35	5.7215	7.170		42.280	

Conclusion:

The results obtained from the pH metric measurements, the values of pKa were found to decrease with increasing temperature. The values of the thermodynamic functions ΔG, ΔH and ΔS were calculated. The values of stability constants reveal that the stability constants decrease with increasing temperature, along with the pKa value.

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