

EVALUATION OF STABILITY CONSTANT AND FREE ENERGY CHANGE (ΔG) OF CD AND IBUPROFEN AT 298⁰K AND 303⁰K PHMETRICALLY AND FIND OUT EFFECT OF TEMPERATURE ON STABILITY CONSTANT

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ABSTRACT

Coordination between cadmium and ibuprofen were evaluated by PH metric method at two temperature 298⁰K and 303⁰K. Ionic strength were kept constant 0.01 M by adding required quantity of KNO₃. The logK and thermodynamic parameter free energy change were evaluated by using Calvin Bjerrum and Irving Rossotti method. Nitrogen gas was passed to the solution to maintain inert atmosphere. Measurement of pH were carried out by using calibrated digital pH meter model 361 and combined glass electrode.

Keywords: Ibuprofen, Cd, PHmetry, Stability Constant(logK), Free Energy Change(ΔG).

Introduction

Ibuprofen was first launched in 1969, (2RS)-1-[4-(2-methyl propyl) phenyl] propionic acid called as ibuprofen which is alternative medicine to aspirin [1]. Complexation of thiosemicarbazone with divalent metal ions were studied potentiometrically [2]. The stability constant and thermodynamic parameters of Cu(II), Ni(II), Co(II), Zn(II) and Mn(II) with α pyridoin 2-methyl thiosemicarbazone and α pyridoin were determined [3]. The formation constant of 1:1 and 1:2 complexation between 2 phenyl-3-(2'-hydroxy-5'-methylbenzylidene)quinazoline-4-(3H)-one and Co(II), Ni(II), Zn(II), Cd(II), Pb(II), Cu(II), Ba(II), Mg(II), Mn(II), Th(IV), UO₂ were determined potentiometrically at 30⁰C potentiometrically [4]. Stability constant of nimesulide and ibuprofen with transition metal ions were determined [5]. The values of logK are determined by Calvin Bjerrum method, used by Irving and Rossotti [6].

Material and Method

Titration were performed in 100ml glass beaker kept in water bath to keep temperature constant. The chemicals used for titration were of analytical grade, solution were prepared in double distill water. pH of the solution were measured by using combined glass electrode and pH-meter model 361. Used pH meter was calibrated by using buffer solution of PH 4.00, 7.00 and 9.2.

Result and Discussion

Experiment involved the titration of three set with NaOH

- 1) SET A- Free acid (0.01M) titrated with NaOH solution.
- 2) SET - Free acid (0.01M) and 0.05M ibuprofen solution titrated with NaOH solution
- 3) SET C- Free acid (0.01M), 0.05 M ibuprofen and 0.01M CdSO₄ solution titrated with NaOH

Ionic strength of each solution maintain constant 0.01 by adding appropriate amount of 1M KNO₃. The titration were performed by placing solution in water bath to maintain temperature [298⁰K and 303⁰K], nitrogen gas was passed through solution for creation of inert atmosphere. From burette 0.1ml NaOH having strength 0.01 M was added after each addition pH of solution were noted and graph were plotted between PH of solution versus NaOH. The curve of acid and ligand deviate at pH 2.5 to 12. The deviation indicate that dissociation of H⁺ from -COOH group of ibuprofen.

Proton Ligand Formation number

Proton ligand formation number (n_A) calculated by Irving Rossotti equation

$$\bar{n}_A = \frac{(E_0 + N)(V_2 + V_1)}{(V_0 + V_1)T^0L}$$

Where

V₀ = initial volume of solution(50ml)

N = normality of sodium hydroxide

T⁰L = Concentration of ligand in 50 ml

Y = number of dissociable proton

V₁ and V₂ = Volume of alkali consumed by acid and alkali on same PH

Metal Ligand Formation Number (n)

'n' is calculated by using following equation,

$$\bar{n} = \frac{(N+E_0)(V_3-V_2)}{(V_0+V_2)(T^0M)} \quad \bar{n} A$$

Where

V₀ = Initial volume of solution (50ml)

N= Normality of sodium hydroxide

T⁰M= Concentration of metal ion

E₀ = Initial concentration of free acid

V₂ and V₃ Volume of NaOH required for Ibuprofen and zinc for same PH.

Cadmium Ibuprofen formation curve

Formation curve are obtained by plotting a graph between n and pH, Metal ligand stability constant log K are obtained by half integral method, at n=0.5 and Point wise method using formula

For calculation of pK

$$\text{Log}(nA/1-nA) = \text{pK} - \text{PH}$$

For calculation metal ligand stability constant log k

$$\text{Log}(n/1-n) = \text{log K} - \text{PL}$$

Free energy change ΔG is calculated by
 $\Delta G = -2.303 RT \log K.$

Table- 1 PK , logK and Free energy change(ΔG)

S.No.	System	Temperature	PK			LogK			Free Energy Change (ΔG) Cal/mole
			Point wise	Half integral	Mean	Point wise	Half integral	Mean	
1	Cd Ibuprofen	298 °K	5.97	6	5.985	7.86	7.6	7.73	-10541.1
2	Cd Ibuprofen	303 °K	5.95	5.9	5.925	6.93	7	6.965	-9657.3

Conclusion

Proton ligand stability constant pK for ibuprofen were evaluated from plotting a graph between nA versus pH at nA = 0.5 and found to be 6 and 5.9 ,pK were also calculated by point wise method ,found to be 5.97 and 5.95,metal ligand stability constant by point wise calculation 7.86 and 6.93 ,by half integral

method 7.6 and 7 and Free energy change ΔG were found to be -10541 and -9657.3[Table 1] at temperature 298 °K and 303 °K respectively .Study suggest that log K decreases with increase in temperature. Negative value of free energy change (ΔG) indicate coordination process is spontaneous.

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