International Journal of Chemical and Physical Sciences, ISSN:2319-6602
IJCPS Vol. 4 Special Issue – NCSC Jan-2015
www.ijcps.org

Studies of Formation Constants of Ethyl-4(2-Hydroxy-Phenyl)-6-Methyl-2-Oxo-1,2,3,4 Tetrahydropyrimidine -5-Carboxylate Complexes with Ca(II), Cu(II) and Ce(III) Metal Ions at 0.1m Ionic Strength pH-Metrycally.

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Abstract

Interaction between Ca(II),Cu(II) and Ce(III) metal ions with Ethyl -4-(2-Hydroxy phenyl)-6-methyl-2-oxo –1,2,3,4-tetrahydropyrimidine-5-carboxylate as antibiotic drug has been investigated at 0.1M ionic strength in 70% dioxane-water medium pH metrically. The values of $\bar{n}_A$ *,* $\bar{n}$*, log*K_1 *and* K_2 *are evaluated and observed that the formation of 1:1 complex and 1:2 complex at* 27^0*C. The correct values of formation constant (log*K_1 *and log*K_2*) are made by making the correction made by Van Uietert.*

Keywords: Ethyl-4(2-hydroxy-phenyl)-6-methyl-2-oxo-1,2,3,4 tetrahydropyrimidine-5-carboxylate,Ca(II),Cu(II) and Ce(III) metal ions, 70% Dioxane-water (solvent).

Introduction

The chemistry of pyrimidines has become increasingly important as a result of recent developments in medicinal chemistry. Pyrimidines are the most important six membered heterocyclic compound. Malhotra and Shrivastava[1] have synthesized some new pyrimidines and determined their characterization and antimicrobial activities. Mohsn[2] have prepared some new pyrimidenes from chalcones containing an Imine group. Andrews and Mansur[3] have synthesized substituted pyrimidine derivatives and study their antifungal activity. Kappe[4] have prepared Dihydropyrimidines, New tricks from old dogs. Patil et al.[5] have synthesized Dihydropyrimidine derivatives using microwave and study their biological screening. No work has been done on metal-ligand stability constants and other physical properties of substituted pyrimidone derivatives . Present work is undertaken to study the stability constants of Ca(II), Cu(II) and Ce(III) metal ion complexes with Ethyl-4-(2-Hydroxy-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidines-5-carboxylate (L_1) at 0.1 M ionic strength.

Experimental

Experimental procedure involves Calvin-Bjerrum titration method, having three types of titration (i)Acid titration,(ii) Acid + Ligand titration and (iii) Acid + Ligand + Metal ions titration. Ionic strength is maintained constants by adding appropriate amount of 1 M KNO_3 solution. Representative graph is shown in fig 1.

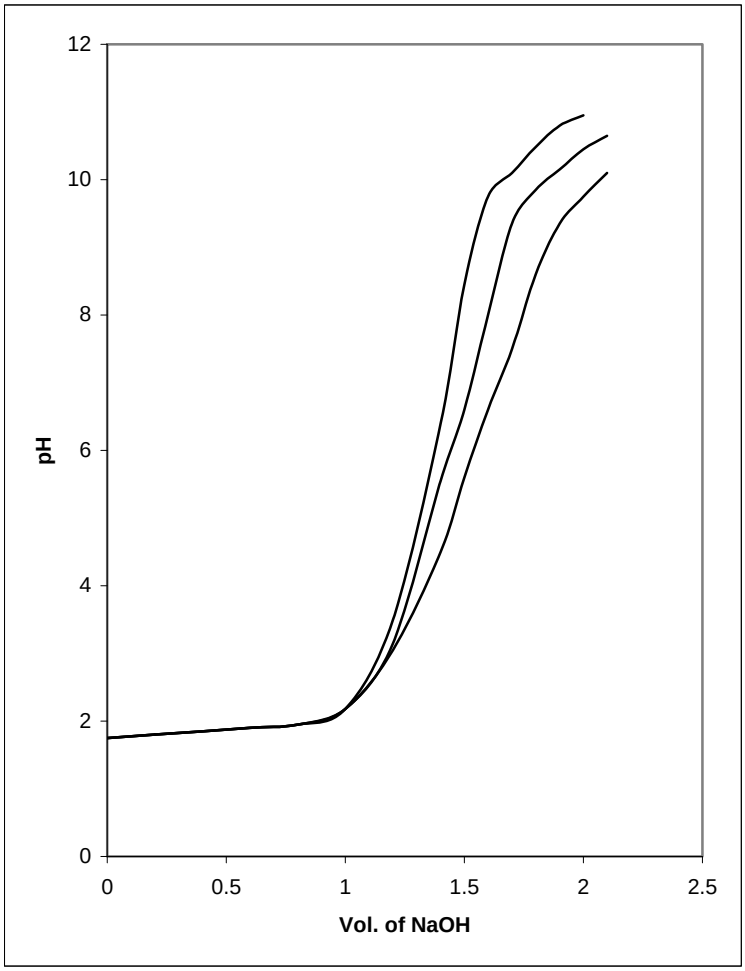

Fig. 1: System- Ca(II)- LIGAND(L1)

Result and Discussion

Deviation between acid curve and ligand curve shows the dissociation of –OH group of ligand and deviation between ligand and metal curve shows the association of ligand species to metal cation for commencement of complex formation. The values of $\bar{n}_A$, $\bar{n}$, $\log K_1$ and K_2 are presented in Table 1 to 5.

Table 1: Determination of $\bar{n}_A$ value system: (L_1)

$T_L^o = 20.00 \times 10^{-4}$ M $V^0 = 12.5$ mL
N = 0.135 M Temp = 27^0C

pH	V_1	V_2	V_2-V_1	$\bar{n}_A$
3.00	1.12	1.20	0.08	0.6770
3.20	1.14	1.22	0.08	0.6774
3.40	1.18	1.26	0.08	0.6783
3.60	1.20	1.28	0.08	0.6788
3.80	1.24	1.33	0.09	0.6397

4.00	1.25	1.34	0.09	0.6400
4.20	1.27	1.37	0.10	0.6005
4.40	1.28	1.39	0.11	0.5609
4.60	1.29	1.40	0.11	0.5612
4.80	1.29	1.40	0.11	0.5612
5.00	1.30	1.41	0.11	0.5615
5.20	1.31	1.42	0.11	0.5619
5.40	1.32	1.44	0.12	0.5224
5.60	1.32	1.44	0.12	0.5225
5.80	1.33	1.45	0.12	0.5227
6.00	1.33	1.45	0.12	0.5228
6.20	1.35	1.47	0.12	0.5234
6.40	1.36	1.48	0.12	0.5238
6.60	1.37	1.50	0.13	0.4844
6.80	1.39	1.52	0.13	0.4852
7.00	1.40	1.54	0.14	0.4460
7.20	1.41	1.55	0.14	0.4464
7.40	1.42	1.56	0.14	0.4468
7.60	1.43	1.57	0.14	0.4473
7.80	1.45	1.59	0.14	0.4480
8.00	1.45	1.59	0.14	0.4480
8.20	1.49	1.63	0.14	0.4496
8.40	1.49	1.63	0.14	0.4496
8.60	1.52	1.67	0.15	0.4115
8.80	1.54	1.69	0.15	0.4123
9.00	1.55	1.71	0.16	0.3736
9.20	1.56	1.72	0.16	0.3741
9.40	1.59	1.75	0.16	0.3754
9.60	1.62	1.80	0.18	0.2988
9.80	1.66	1.84	0.18	0.3008
10.00	1.70	1.90	0.20	0.2253

Table 2 : Determination of $\bar{n}$ values system: Ca(II) – L_1

$E^0 = 1.00 \times 10^{-2}$ M $T_L^0 = 20.00 \times 10^{-4}$ M $T_m^0 = 4.00 \times 10^{-4}$ M
$V^0 = 12.5$ mL N = 0.135 M Temp = 27^0 C

pH	V_2	V_3	V_3-V_2	$\bar{n}$
4.00	1.34	1.35	0.01	0.1986
4.20	1.37	1.38	0.01	0.1982
4.40	1.39	1.40	0.01	0.1979
4.60	1.40	1.41	0.01	0.1978
4.80	1.40	1.42	0.02	0.3956
5.00	1.41	1.43	0.02	0.3953
5.20	1.42	1.45	0.03	0.5926
5.40	1.44	1.47	0.03	0.5918
5.60	1.44	1.48	0.04	0.7890
5.80	1.45	1.50	0.05	0.9856
6.00	1.45	1.51	0.06	1.1827
6.20	1.47	1.54	0.07	1.3779
6.40	1.48	1.59	0.11	2.1638
6.60	1.50	1.61	0.11	2.1607
6.80	1.52	1.64	0.12	2.3537

Table 3 : Determination of $\bar{n}$ values system : Cu (II) – L_1

$E^0 = 1.00 \times 10^{-2}$ M $T_L^0 = 20.00 \times 10^{-4}$ M $T_m^0 = 4.00 \times 10^{-4}$ M
$V^0 = 12.5$ mL N = 0.135 M Temp = 27^0 C

pH	V_2	V_3	V_3-V_2	$\bar{n}$
3.6	1.28	1.30	0.02	0.3991
3.8	1.33	1.35	0.02	0.3976
4.0	1.34	1.37	0.03	0.5960
4.2	1.37	1.40	0.03	0.5948
4.4	1.39	1.42	0.03	0.5939
4.6	1.40	1.45	0.05	0.9892
4.8	1.40	1.47	0.07	1.3848
5.0	1.41	1.48	0.07	1.3838
5.2	1.42	1.50	0.08	1.5804

5.4	1.44	1.52	0.08	1.5781
5.6	1.44	1.53	0.09	1.7754
5.8	1.45	1.54	0.09	1.7741
6.0	1.45	1.55	0.10	1.9713
6.2	1.47	1.58	0.11	2.1653
6.4	1.48	1.59	0.11	2.1638
6.6	1.50	1.61	0.11	2.1607

Table 4: Determination of values system: Ce(III) – L_1

$E^0 = 1.00 \times 10^{-2}$ M $T_L^0 = 20.00 \times 10^{-4}$ M $T_m^0 = 4.00 \times 10^{-4}$ M
$V^0 = 12.5$ mL N = 0.135 M Temp = 27^0 C

pH	V_2	V_3	V_3-V_2	$\bar{n}$
2.60	1.18	1.200	0.020	0.4204
2.80	1.20	1.225	0.025	0.5018
3.00	1.20	1.240	0.040	0.8029
3.20	1.22	1.260	0.040	0.8017
3.40	1.26	1.320	0.060	1.1939
3.60	1.28	1.340	0.060	1.1939
3.80	1.33	1.390	0.060	1.1930
4.00	1.34	1.410	0.070	1.3908
4.20	1.37	1.440	0.070	1.3878
4.40	1.39	1.460	0.070	1.3858
4.60	1.40	1.470	0.070	1.3848
4.80	1.40	1.480	0.080	1.5827
5.00	1.41	1.500	0.090	1.7792
5.20	1.42	1.510	0.090	1.7780
5.40	1.44	1.530	0.090	1.7754
5.60	1.44	1.550	0.110	2.1700

It could be seen from Table 4, that there is considerable difference between logK values of Ce(III)-L_1complexes. This shows the formation of stepwise complexes. In case of Cu(II)-L_1 and Ca(II)-L_1 complexes, there is minimum difference between log K values, this shows the formation of simultaneous complexes.

Table 5: Metal–Ligand stability constants (log K_1 and K_2)

System	Log K_1	Log K_2
Ca(II) –L_1	3.894	2.898
Cu(II) – L_1	5.190	4.352
Ce(III) – L_1	7.342	4.401

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