ISSN 2348-1218 (print)
International Journal of Interdisciplinary Research and Innovations ISSN 2348-1226 (online)
Vol. 10, Issue 4, pp: (40-45), Month: October 2022 - December 2022, Available at: www.researchpublish.com

Chemical kinetic of Dy^{3+} rare metal Complex with Benzoxazole Derivative

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DOI: https://doi.org/10.5281/zenodo.7320022

Published Date: 14-November-2022

Abstract: **The combination of some rare metal ions with an important 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide (BSPA) ligand to form coordination compounds is an important area of current research. Less explored biologically important 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide ligand is allowed to react with solution of some rare metal perchlorates and attempt has been made to synthesize solid 2-(1,3-benzoxazole -2-yl-sulfanyl)-N-phenyl acetamide complexes. These 2-(1,3-benzoxazole-2-yl-sulfanyl)-N-phenyl acetamide complexes are subjected to antimicrobial activity of these complexes has been evaluated by standard methods and attempts have been made to correlate structural characteristics with properties of these 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide complexes.**

Keywords: **Spectroscopic characterization, 2-(1,3-Benzoxazole-2-yl-sulfanyl)-N-phenyl acetamide(BSPA) complex, catalysis, antimicrobial activity.**

1. INTRODUCTION

1.1Chemical Kinetic

Reaction 1:-

The experiment was carried out with two reacting species $K_2S_2O_8$ and KI using their equal concentrations.[1-3] This reaction is carried out as as under gives the kinetic data without addition of any catalyst. [1-3]

Table 1: Reaction kinetics (without catalyst):

Reaction of : $K_2S_2O_8$ + KI + Methanol

Concentration : (0.0227M) (0.0227M) --

Volume : 50ml 50ml 10ml (t_∞ =113.5 ml)

Time t (min.)	Burette reading X (ml)	K = 1/at * X/(a-x) ($lit.mol^{-1}\ min^{-1}$)
5	3.2	4.20×10^{-5}
10	3.7	2.44×10^{-5}
15	4.1	1.80×10^{-5}
20	4.6	1.52×10^{-5}
25	5.0	1.33×10^{-5}
30	5.5	1.22×10^{-5}

average k = 2.085×10^{-5}

a=b=initial concentrations of reactants = 113.5 ml

t_∞ =113.5 ml

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Reaction:-

$$K_2S_2O_8 + 2KI \rightarrow 2K_2SO_4 + I_2$$

$$2Na_2S_2O_3 + I_2 \rightarrow 2NaI + Na_2S_4O_6$$

Table 2: Reaction kinetics table without catalyst

Reaction of : $KBrO_3$ + KI + HCl + Methanol

Concentration : (0.0096M) (0.0096M) --

Volume : 25ml 25ml 10ml (t∞ =25ml)

Time t (min.)	Burette reading X (ml)	K = 1/at * X/(a-x) ($lit.mol^{-1}\ min^{-1}$)
5	6.9	3.04×10^{-3}
10	7.4	1.68×10^{-3}
15	7.7	1.18×10^{-3}
20	8.6	1.04×10^{-3}
25	9.0	0.9×10^{-3}
30	9.5	0.81×10^{-3}

average k = 1.44×10^{-3}

a=b=initial concentrations of reactants = 25 ml

t∞ = 25ml

Reaction :-

$$KBrO_3 + HCl \longrightarrow KCl + HBrO_3$$

$$KI + HCl \longrightarrow KCl + HI$$

$$HBrO_3 + 6HI \longrightarrow HBr + 3H_2O + 3I_2$$

$$I_2 + 2Na_2S_2O_3 \longrightarrow 2NaI + Na_2S_4O_6$$

Table 3: Reaction kinetics table without catalyst

Reaction of : H_2O_2 + KI + H_2SO_4 + Methanol

Concentration : (0.0091M) (0.0091M) --

Volume : 10ml 10ml 10ml (t∞ =50ml)

Time t (min.)	Burette reading X (ml)	K = 1/at * X/(a-x) ($lit.mol^{-1}\ min^{-1}$)
5	1.2	9.8×10^{-5}
10	1.7	7.03×10^{-5}
15	2.3	6.42×10^{-5}
20	2.9	6.15×10^{-5}
25	3.4	5.83×10^{-5}
30	3.8	5.48×10^{-5}

average k = 6.78×10^{-5}

a=b=initial concentrations of reactants = 50 ml

t∞ =50ml

Reaction:-

$$H_2O_2 + 2HI \longrightarrow 2H_2O + I_2$$

$$I_2 + 2Na_2S_2O_3 \longrightarrow 2NaI + Na_2S_4O_6$$

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The percentage increase in reaction rates, as shown in table 11, is calculated as shown below.

$$\text{Percentage Increase} = \frac{\text{Reaction rate with catalyst -- Reaction rate without catalyst}}{\text{Reaction rate without catalyst}} \times 100$$

Table 4: Overall Results of catalytic activity for complexes of Dy^{3+} metal ions

Reactions	k without Complexes	k with Dy -BSPA (1%)	% Increase reaction rate at T = 300K Dy-BSPA
$K_2S_2O_8$ + KI	2.085×10^{-5}	5.7×10^{-5}	173
$KBrO_3$ + HI	1.44×10^{-3}	4.15×10^{-2}	2781.94
H_2O_2 + HI	6.78×10^{-5}	4.05×10^{-4}	497.34

k = reaction rate constant for the second order reaction, 1% complex = 1 % molecular weight of the complex

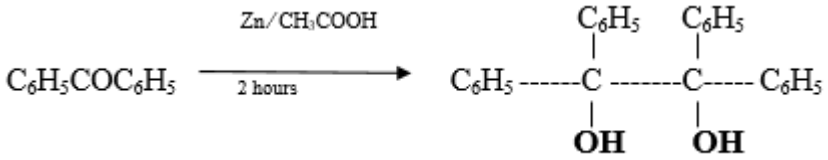
1 % MW of Dy-BSPA = **0.0131 gm** Dy-BSPA ≡ **0.043 % of mole of $K_2S_2O_8$ ≡ 0.104 % of mole of $KBrO_3$ ≡ 0.11 % of mole of H_2O_2,**

1.2 Catalysis of Organic Reaction:-

The catalyst is one type of molecule which facilitates the reaction In homogeneous catalysis, the reactant (s) coordinate[4-6] to the catalyst (or vice versa), are transformed to product, which are then released from the catalyst [4-6].

A mixture of benzophenone (7.5 gm, 0.041 mole) zinc dust (4 gm) glacial acetic acid (110 ml) and water (22 ml) is refluxed for 2 hours. The solution is filtered (if necessary) and cooled. The separated benzpinacol is filtered and crystallized from glacial acetic acid. The yield is 4.5 gm (30%).

The product melting point was 188-189 ^{0}C.[7-9]



Benzophenone **Benzpinacol**

Table 5: Percentage yield without catalyst for different reaction times

No	Temperature	% yield without catalyst (for 3 hours reaction)	% yield without catalyst (for 2 hours reaction)
1	368 K	55.55%	30.00 %

Table 6: Percentage yield with catalyst metal complexes (for 2 hours reaction time) Temperature = 368 K (yield without catalyst is 30%)

Complexes	% yield for 1%catalyst addition	% yield for 5%catalyst addition	% yield for 10%catalyst addition
Tb-BSPA	27.26	45.03	76.09

1%MW of complex (catalyst) ≡ 0.0243 % of mole of benzophenone

5%MW of complex (catalyst) ≡ 0.121 % of mole of benzophenone

10%MW of complex (catalyst) ≡ 0.243 % of mole of benzophenone

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1.3 Results and Discussion of catalysis experiments:-

The benzpinacol formation reaction was carried out with identical conditions. Here, Dy-BSPA also successfully acted as homogeneous catalysts. It was observed that addition of the complex in catalytic amounts increased the yield. Dy-BSPA. [10-13]The most possible cause of lower yield on addition of 1% catalyst in each case seems to be due to the solvent methanol. When Eu^{3+}complex were added in the reaction system,[5] the yield increased[10-13] significantly and hence there is a great chance that some of these complexes can increase the yield of an industrially important reaction by saving time, energy and consequently money. [10-13]

2. ANTIBACTERIAL ACTIVITY

This part deals with the in-vitro screening of the complexes for antibacterial activity. The species *S.aureus*, *E.coli*, *S.Phyogenus* and *P.Aeruginosa* have been taken for the antibacterial activities[14]. Agar-cup method was carried out for the in-vitro screening for antibacterial activity.[14] The results of the compounds employed for antibacterial screening are mentioned in following Table.

Table 7: Antimicrobial activity of Standard drugs

STANDARD DRUGS				
MINIMUM INHIBITION CONCENTRATION (µg/ml)				
DRUG	***E.coli***	***P.aeruginosa***	***S.aureus***	***S.phyogenus***
µg/ml	**MTCC 443**	**MTCC 1688**	**MTCC 96**	**MTCC 442**
GENTAMYCIN	0.05	1	0.25	0.5
AMPICILLIN	100	--	250	100
CHLORAMPHENICOL	50	50	50	50
CIPROFLOXACIN	25	25	50	50
NORFLOXACIN	10	10	10	10

Table 8: Antibacterial activity of BSPA Ligand with Dy^{3+} Complexes

ANTIBACTERIAL ACTIVITY TABLE					
MINIMUM TNHIBITION CONCENTRATION µg/ml					
SR NO	**CODE NO**	***E.coli*** **MTCC 443**	***P.aeruginosa*** **MTCC 1688**	***S.aureus*** **MTCC 96**	***S.phyogenus*** **MTCC 442**
1	BSPA	200	200	100	125
2	Dy-BSPA	264	208	129	102

Comparison of antimicrobial activity of produced compounds with that of standard antimicrobial drugs reveals that[9] the synthesized compounds show moderate to good activity against all four bacterial strains.

3. ANTIFUNGAL ACTIVITY

This part deals with the in-vitro screening of newly prepared compounds for activity. The species *C. albicans*, *A.niger*, *A.clavatus* have been taken for the antifungal activities. Agar-cup method was used for the in-vitro screening for antifungal activity.[15-16] The results of the compounds for antifungal screening are mentioned in following table.

Table 9: Antifungal Activity of Standard Drugs

MINIMAL INHIBITION CONCENTRATION Standard drugs			
DRUGS	***C.albicans***	***A.niger***	***A.clavatus***
	MTCC 227	**MTCC 282**	**MTCC 1323**
mg/ml			
NYSTSTIN	**100**	**100**	**100**
GRESEOFULVIN	**500**	**100**	**100**

Table 10: Antifungal activity of BSPA ligand with Dy3+Complex

ANTIFUNGAL ACTIVITY TABLE				
MINIMAL FUNGICIDAL CONCENTRATION µg/ml				
SR NO	**CODE NO**	***C.albicans* MTCC 227**	***A.niger* MTCC 282**	***A.clavatus* MTCC 1323**
1	BSPA	500	1000	>1000
2	Dy-BSPA	255	502	505

Comparison of antimicrobial activity of produced compounds with that of standard antimicrobial drugs reveals[17-18] that the prepared complexes show moderate to good activity against all three fungal strains.

4. RESULTS AND DISCUSSION OF ANTIMICROBIAL ACTIVITIES

Results of antibacterial activities of the complexes suggested that complex exhibited equal activity as standard drug ampicillin towards *E.coli.* against *S.aureus* [19-21]showed equal activity and greater activity was exhibited by Dy-BSPA complex compared to standard ampicillin drug. The remaining antibiotics exhibited greater activities[19-21] compared to the antibacterial performance of the two complex. The antifungal activities of the complex were found to be less than that of standard antifungal antibiotic drugs. [19-21]

5. CONCLUSION

Rare metals and their compound possess a wide variety of properties. With a view to exploring them, two lanthanide ions and the ligand BSPA were chosen. The selection of the BSPA ligand was based upon the possibility of complex formation through donation of electron pair by any two/ three/ more atoms out of two nitrogen atoms, two oxygen atoms and one sulphur atom.

ACKNOWLEDGEMENT

Authors thank to Hemchandracharya North Gujarat University, Patan, India for supply chemical, A grade glass were and wonderful laboratory provide. We are thankful to Central Instrumental maintenance Facilities (CIMF) Laboratory Hemchandracharya North Gujarat University, Patan, India to facilities of Spectral analysis.

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