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Chemical kinetic activity of Iridium rare metal Complex with Banzoxazole Derivative

[1]Dr. H. D. Chaudhari, [2]Dr. Haresh R.Patel

[1] Department of Chemistry, Hemchandracharya North Gujarat University, Patan,

[2]Department of Chemistry, Khedbrahma Campus, Hemchandracharya North Gujarat University, Vadali, Gujarat

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Abstract: **The combination of Iridium 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, chemical kinetic activity, catalysis.**

1. CHEMICAL KINETIC ACTIVITY

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 X 10^{-5}
10	3.7	2.44 X 10^{-5}
15	4.1	1.80 X 10^{-5}
20	4.6	1.52 X 10^{-5}
25	5.0	1.33 X 10^{-5}
30	5.5	1.22 X 10^{-5}

average k = 2.085 x 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 ($t\infty$ =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

$t\infty$ = 25ml

Reaction :-

$KBrO_3 + HCl \rightarrow KCl + HBrO_3$

$KI + HCl \rightarrow KCl + HI$

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

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

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 ($t\infty$ =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

$t\infty$ =50ml

Reaction:-

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

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

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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 Iridium metal ions

Reactions	k without Complexes	k with Ir –BSPA (1%)	% Increase reaction rate at T = 300K Ir -BSPA
$K_2S_2O_8$ + KI	**2.085 X 10^{-5}**	**3.8 X 10^{-5}**	**82.25**
$KBrO_3$ + HI	**1.44 X 10^{-3}**	**2.30 X 10^{-2}**	**1497.22**
H_2O_2 + HI	**6.78 X 10^{-5}**	**2.25 X 10^{-4}**	**231.85**

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

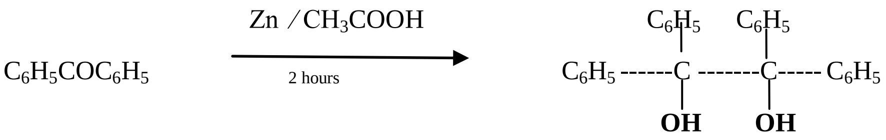
1 % MW of Ir-BSPA = 0.0131 gm Ir-BSPA ≡ 0.043 % of mole of $K_2S_2O_8$ ≡ 0.104 % of mole of $KBrO_3$ ≡ 0.11 % of mole of H_2O_2,

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

Sr. 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**
Ir-BSPA	21.65	36.81	54.68

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

3. RESULTS AND DISCUSSION OF CATALYSIS EXPERIMENTS

The benzpinacol formation reaction was carried out with identical conditions. Here, Ir -BSPA also successfully acted as homogeneous catalysts. It was observed that addition of the complex in catalytic amounts increased the yield. Ir -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 Iridium metal 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]

4. CONCLUSION

Rare metals and their compound possess a wide variety of properties. With a view to exploring them, two Iridium 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.

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