IOSR Journal of Applied Chemistry (IOSR-JAC)
e-ISSN: 2278-5736.Volume 13, Issue 11 Ser. II (November. 2020), PP 21-24
www.iosrjournals.org

Quantitative Structure–Activity Relationshipof Fungicidalon Water Pollution:Study of Tetramethyl thiuram disulphide (Thiram)& Zinc dimethyl dithiocarbamate (Ziram)

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Abstract: *The current study shows that the effect of variables was now studied in the order to establish the reaction conditions. As representative test sample Ziram (tech.) was chosen for Dithiocarbamate compounds. During the studies of effect of reaction time keeping the amount of Ziram (tech.), the concentration of acetic acid and Chloramine-T reagent as constant.*

Background*: The toxicity and mechanism of action of dialkyl dithiocarbamates and mono alkyl dithiocarbamates are discussed in detail by various workers[5-15]. The toxicological effects like acute toxicity[16], chronic toxicity[17], reproductive effects[18], teratogenic effects[19], organ toxicity[20], mutagenic effects[21], carcinogenic effects[23], ecological effects[24] and environmental fate[24-25] of Dithiocarbamate compounds have also been discussed.*

Materials and Methods*: In a 100 ml Erlenmeyer flask, Aliquot containing 1-5 mg of the sample were taken. Further 10 ml of glacial acetic acid and 10 ml of 0.2 N Chloramine-T were now added to it. The contents were now shaken well. At room temperature (27°C), It is allowed to react for 10 minutes. 10 ml of 10% potassium iodide solution was added after the reaction was over. It is now the contents were alos allowed to the stand for only one minute. With standard 0.2 N sodium thiosulphate solution, the liberated iodine was now titrated using starch as an indicator. Using all the reagents except the sample, a blank experiment was also run under the similar conditions. For the sample was now calculated with the difference in readings of sodium thiosulphate solution, the amount of Chloramine- T consumed for the blank and the sample experiment.*

Results*: For the determination of the concentration of some fungicidal dithiocarbamate compounds, the effect of following variables was mainly studied. As a test sample Ziram (tech.) is taken. Effect of the Reaction Time was measured. For the amount of Ziram (tech.), the concentration of acetic acid and Chloramine-T as constant. The reaction time was varied from 1-15 minutes. By titrating the reaction mixture using standardized (0.2 N) sodium thiosulphate solution along with starch and potassium iodide as indicator, the unutilized Chloramine-T was mainly determined. It was found that within 10 minutes the recovery of Ziram (tech.) becomes very much constant. By allowing more reaction time, the value does not change generally significantly. The tendency of positive error increases by increasing the reaction time.*

Conclusion: *The current study shows that the effect of variables was now studied in the order to establish the reaction conditions. As representative test sample Ziram (tech.) was chosen for Dithiocarbamate compounds. During the studies of effect of reaction time keeping the amount of Ziram (tech.), the concentration of acetic acid and Chloramine-T reagent as constant.*

Key Word*: Quantitative Structure–Activity Relationship, Fungicidal, Water Pollution, Tetramethyl thiuram disulphide (Thiram), Zinc dimethyl dithiocarbamate (Ziram)*

Date of Submission: 06-11-2020 Date of Acceptance: 19-11-2020

I. Introduction

The toxicity and mechanism of action of dialkyl dithiocarbamates and mono alkyl dithiocarbamates are discussed in detail by various workers[5-15]. The toxicological effects like acute toxicity[16], chronic toxicity[17], reproductive effects[18], teratogenic effects[19], organ toxicity[20], mutagenic effects[21], carcinogenic effects[23], ecological effects[24] and environmental fate[24-25] of Dithiocarbamate compounds have also been discussed. Because of the great insecticidal and fungicidal importance, the analysis of Dithiocarbamate compounds need prime attention. Mckinly and Magarvey[56] reported paper chromatography procedure for the resolution of some dithiocarbamate compounds. Henriet and Co-workers[57] reported a standardised method for analysis of dithiocarbamate residue in lettuces. Sheinina and Co-workers[58] used thin layer chromatography for the determination of thiram in cotton seed with hexane. Strigina and Co-workers[59] reported complexometric determination of TMTD. Butler and Co-workers[60] reported a trace analysis of thiram by microcoulometry. Lukashevich and Co-workers[61] reported a method for determining the working concentrations of TMTD

(thiram) and the quality of tuber disinfection. Several other liquid chrornatography[62], titrimetric[63], potentiomertic[64], spectrophotometric[65-66] and high-performance liquid chromatographic[67-69] procedures for the determinations of dithiocarbamate compounds are also reported.

Zinc dimethyl dithiocarbamate (Ziram) for testing quantitative validity of the reaction, was mainly taken as the test sample. The contents were shaken well. At room temperature for different intervals of reaction time, it is further allowed to react with varying concentration of Chloramine- T reagent. The unconsumed Chloramine-T was generally determined iodometrically after the reaction was over. The stoichiometry of the reaction was generally established for each sample. There is a possible course of reaction suggested. Using all the reagents except the sample, there is a blank experiment run under similar conditions. The estimation of other dithiocarbamate compounds in more technical form and in their formulations were carried out on the basis of reaction conditions developed for Zinc dimethyl dithiocarbamate (Ziram).

II. Material and Methods

In a 100 ml Erlenmeyer flask, Aliquot containing 1-5 mg of the sample were taken. Further 10 ml of glacial acetic acid and 10 ml of 0.2 N Chloramine-T were now added to it. The contents were now shaken well. At room temperature (27°C), It is allowed to react for 10 minutes. 10 ml of 10% potassium iodide solution was added after the reaction was over. It is now the contents were alos allowed to the stand for only one minute. With standard 0.2 N sodium thiosulphate solution, the liberated iodine was now titrated using starch as an indicator. Using all the reagents except the sample, a blank experiment was also run under the similar conditions. For the sample was now calculated with the difference in readings of sodium thiosulphate solution, the amount of Chloramine- T consumed for the blank and the sample experiment.

III. Result and Discussion

For the determination of the concentration of some fungicidal dithiocarbamate compounds, the effect of following variables was mainly studied. As a test sample Ziram (tech.) is taken. Effect of the Reaction Time was measured. For the amount of Ziram (tech.), the concentration of acetic acid and Chloramine-T as constant. The reaction time was varied from 1-15 minutes. By titrating the reaction mixture using standardised (0.2 N) sodium thiosulphate solution along with starch and potassium iodide as indicator, the unutilized Chloramine-T was mainly determined. It was found that within 10 minutes the recovery of Ziram (tech.) becomes very much constant. By allowing more reaction time, the value does not change generally significantly. The tendency of positive error increases by increasing the reaction time.

The effect of varying the concentration of Chloramine-T was generally studied keeping reaction time, the amount of glacial acetic acid and Ziram (tech.) as constant. 10 ml of varying concentration (0.01 to 0.50N) of Chloramine-T reagent was allowed to react with 9.875 mg of the sample.

The unreacted Chloramine-T was determined iodometrically and the recovery of the sample was calculated. In the determination of the Ziram (tech.), variation in the volume of Chloramine-T reagent (0.2 N) was also found. 10 ml of 0.2 N Chloramine-T reagent gives just accurate results. The same result was also very much obtained in the determination of the other fungicidal samples.

Keeping reaction time, the concentration of Chloramine-T and the amount of Ziram (tech.) as constant, the 5% concentration of the acetic acid to glacial was varied. The results were nicely noted (Table-4).

By mixing distilled water in glacial acetic acid, the dilute solutions of the acetic acid were found. Glacial acetic acid gives stoichiometric and quantitative results with Ziram as indicated in the table. In case of other dithiocarbamate compounds, the same results were generally obtained. In the absence of glacial acetic acid, the reaction was also carried out, the results are concordant and inaccurate values were not mainly obtained.

The reaction temperature was mainly varied from 0°C to 100°C keeping all other conditions constant. The recovery of the Ziram (tech.) was mainly calculated (Table-6). Within 10 minutes at room temperature (27°C), the reaction was completed. Inaccurate results found for the heating of the reaction mixture. At room temperature, the reaction is carried out since the reagent decomposes on heating. At the lowest temperature generally, there is no reaction. However, if the reaction temperature is generally lowered to freezing point (DOC) it results the reactivity of the reagent is retarded.

On an accurate scale and testing the utility of the sample for evaluating results, a large number of experiments were now carried out and the different variables were nicely calculated.

Standard deviation, Percentage error and the coefficient of variation was nicely calculated for the each determination with the each technical sample and their formulations. The standard deviation was precisely calculated by the following expression;

SD (Standard deviation) = $\sqrt{\frac{(x_1-\bar{x})^2+(x_2-\bar{x})^2+\ldots\ldots+(x_n-\bar{x})^2}{n-1}}$

Where,

$\bar{x}$ = Average value or Mean value of the amount obtained by calculation.

x_1 x_2, x_3……..x_n are the amount obtained from the calculations

and n = Number of the observations.

IV. Conclusion

The current study shows that the effect of variables was now studied in the order to establish the reaction conditions. As representative test sample Ziram (tech.) was chosen for Dithiocarbamate compounds. During the studies of effect of reaction time keeping the amount of Ziram (tech.), the concentration of acetic acid and Chloramine-T reagent as constant.

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Santosh Kumar Srivastwa, et. al. "Quantitative Structure–Activity Relationshipof Fungicidalon Water Pollution:Study of Tetramethyl thiuram disulphide (Thiram)& Zinc dimethyl dithiocarbamate (Ziram)." *IOSR Journal of Applied Chemistry (IOSR-JAC)*, 13(11), (2020): pp 21-24.