

CHAPTER IV

CONCLUSION

4.1 Conclusion

The aim of this work was to synthesize 4-chloro-5-(3',4'-dinitrophenyl)-2-(4-vinylphenyl)oxazole. The preparation method, chosen by considering the available chemicals, equipments and glasswares, was devised to 8 steps. The optimum conditions for each step were studied in order to get good yields. The results summary of are shown in Table 4.1. While the optimum condition were not established for the synthesis of the target compound, spectroscopic data indicates that the target has, in fact, been achieved.

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Table 4.1 The starting material, physical properties and yield of each step .

Product	Starting Material	Physical Appearance	Yield
(2)	(1)	pale yellow solid, m.p.147°C, lit 146°C [20].	92%
(3)	(2)	yellow brown needle crystal, m.p. 60°C, lit 54-57°C [20].	96%
(4)	(3)	light yellow crystal, m.p.161°C,lit 165°C [20].	89%
(5)	(4)	transparent yellow brown crystal, m.p. 50.6°C,lit50-51°C[21]	99%
(6)	(5)	brown red viscous liquid ^a (new compound)	20.2 g based (5)
(7)	(6) and 4-ethylbenzaldehyde	bright yellow needle crystal, m.p.133.8°C (new compound)	8.2 g based (6)
(8)	(7)	pale yellow needle crystal ^b , m.p.180.6°C (new compound)	6.4 g based (7)
(9)	(8)	pale green yellow solid ^{a,c} , m.p.141.8°C (new compound)	0.7 g based (8)

Remark : a) The purification method of this compound was not achieved in this study.

b) mixed isomer.

c) Optimum synthesis condition to obtain the highest yield requires further studies.

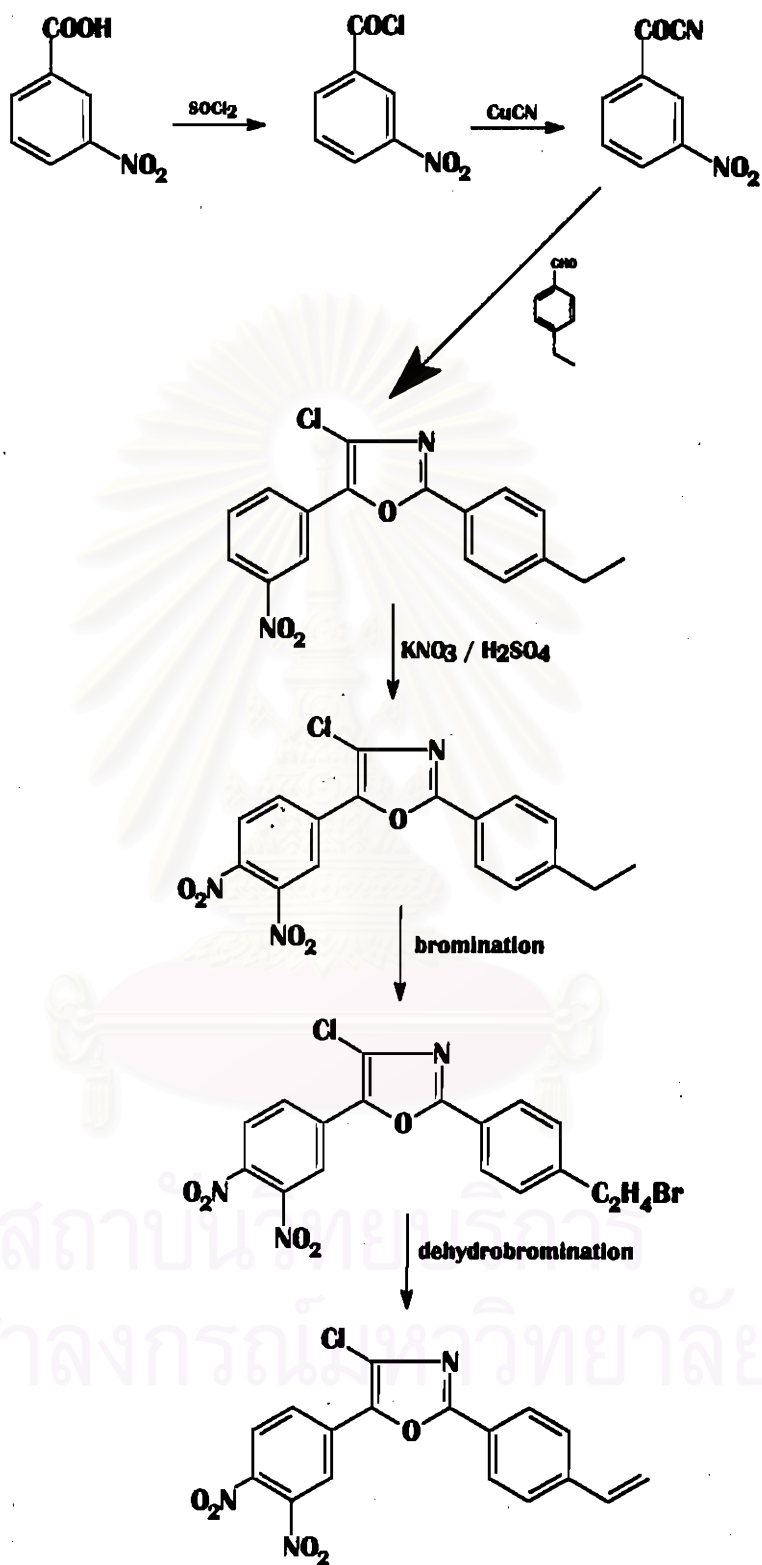
4.2 Difficulties Encountered in This Work

Dinitroaromatic compounds are thermally labile and hence are often used as explosives. For this reason purification by distillation was not attempted. Crystallization was also difficult as the dinitroaroyl halides were very sensitive to moisture.

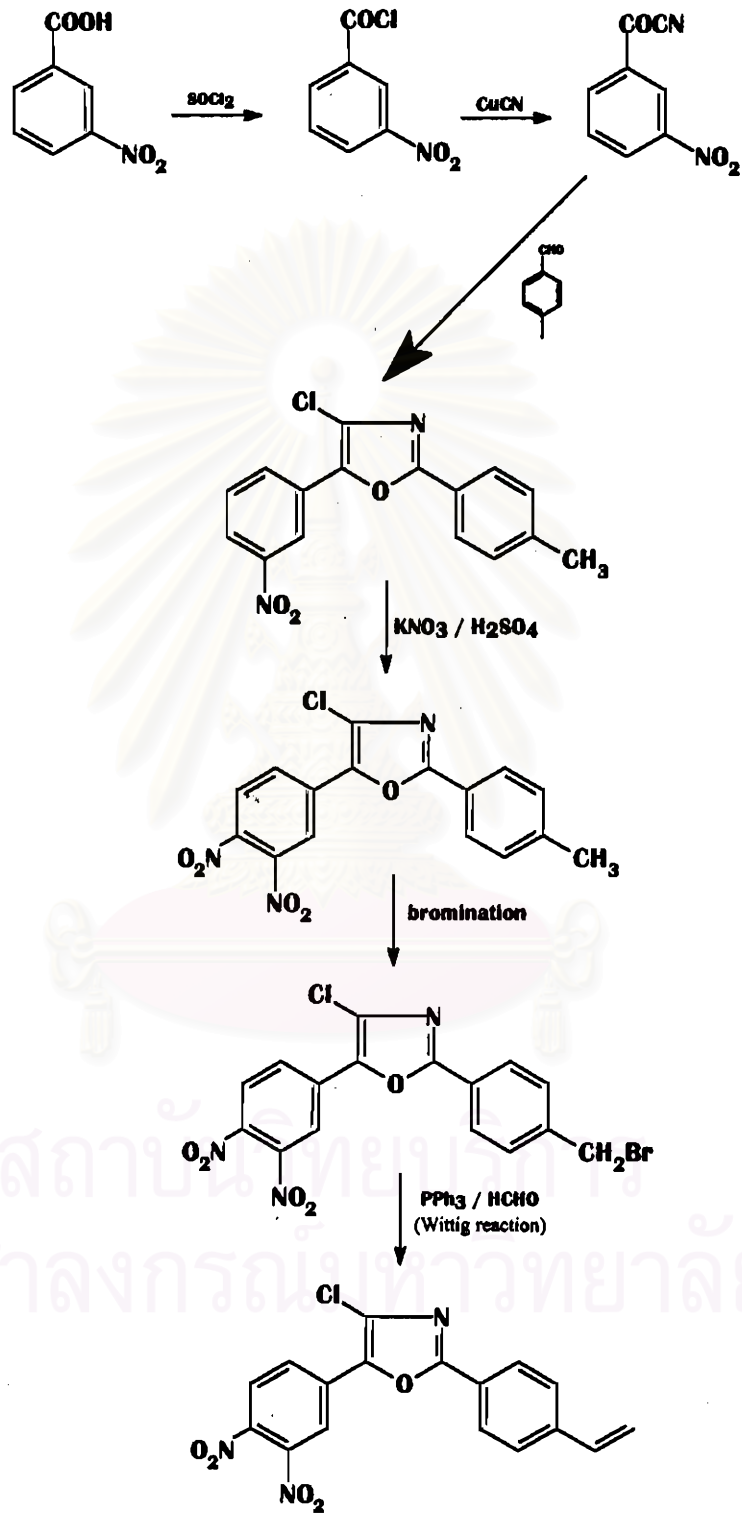
4.3 Suggestion for Further Work

3-Nitrobenzoyl chloride should be used as a starting material to replace 3,4-dinitrobenzoyl chloride in the synthesis of (6) because it is less reactive than 3,4-dinitrobenzoyl chloride so that the 3-nitrobenzoyl chloride should be easier to purify. It could be readily converted to the nitrile, then to the oxazole. Aryl oxazoles nitrate easily converted to dinitrooxazole derivative if $\text{KNO}_3 / \text{H}_2\text{SO}_4$ is used. The aliphatic side-chain of aryl oxazole nitrate won't be oxidized (see Scheme 4.1). In addition, Wittig reaction may be used to substitute in the dehydrobromination step while the starting materials in Ternai synthesis step should be 3,4-dinitrobenzoyl cyanide or 3-nitrobenzoyl cyanide and 4-methylbenzaldehyde (see Scheme 4.2).

The compound (10) should be used as one of comonomer together with styrene or methyl methacrylate. The copolymerization of those comonomers should result in copolymer and its property should be examined. In this work the compound (10) synthesized was not pure so that the improvement of the dehydrobromination step should be carried out and it is purified will prior to copolymerization.



Scheme 4.1



Scheme 4.2