

## Synthesis and Crystallography of some Polychlorinated Naphthalenes

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Polychlorinated naphthalenes (PCN), as polychlorinated biphenyls (PCB), have mainly been used in the electrical industry due to the high degree of chemical and thermal stability. PCN have also been used as additive in oils to clean sludge and petroleum deposits from engines and due to its flame resistance, fungicidal and insecticidal properties they have been used to impregnate wood, paper and textiles<sup>1</sup>. The PCN products are complex mixtures of chlorinated naphthalenes with various degree of chlorination<sup>1</sup>. Toxicological studies of the products indicate that the toxicity increases with the degree of chlorination up to the penta- and the hexachlorinated naphthalenes, that have been associated with skin problems (chloracne) and liver damages<sup>1,2</sup>. The last few years PCN have more and more been recognized as a potentially serious environmental problem. In the Swedish environment tetraCNs and a few pentaCNs and hexaCNs have been reported from analyses of fish and mammalian samples<sup>3</sup>.

The aim of the present study have been to find synthetic routes to individual PCN isomers in order to make them available for analytical and toxicological studies and to determine physical properties of these compounds. During the progress of the work we have synthesized several PCN congeners via principally two pathways; (I) dehalogenation by lithium aluminium hydride (LAH) and (II) chlorination of dinitronaphthalenes with subsequent substitution of the nitro-groups with chlorine atoms (the Ponomarenko reaction), cf. Fig. 1<sup>4,5</sup>. Three of the synthesized compounds, 1,2,3,4,6,7-, 1,2,3,5,6,7- and 1,2,4,5,6,8-hexachloronaphthalene, have been studied with x-ray crystallography. The three compounds were all find to be co-planar.

The possibility to prepare certain PCN congeners via the nitration of a chlorinated naphthalene isomer and subsequent substitution of the nitro-group with a chlorine atom is presently beeing investigated.

### Acknowledgement

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References

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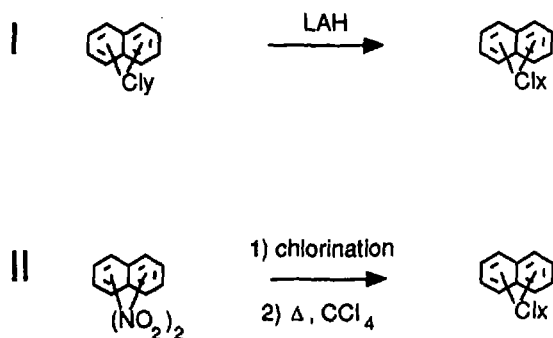


Fig. 1 General pathways for the synthesis of PCN congeners.