Nature of Invention: Chemical molecule and synthesis route

Applicant: UltravioletChemicals

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Chemical Formula: $C_{12}H_{14}O_4$

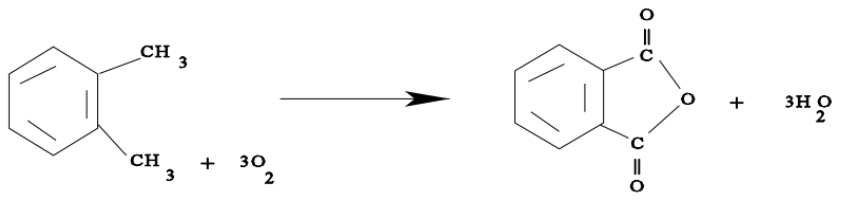
Chemical Name: Diethyl Phthalate

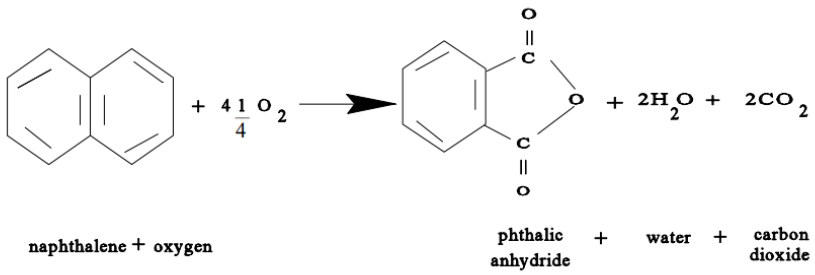
Chemical synthesis routes:

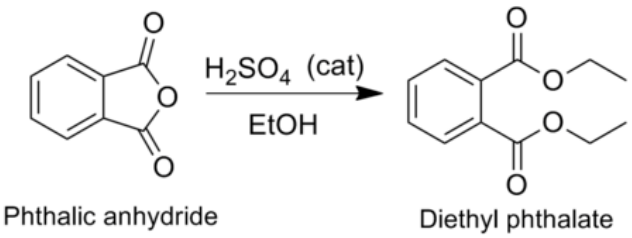
a. Diethyl phthalate is produced by the reaction of phthalic anhydride with ethanol in the presence of concentrated sulfuric acid catalyst (HSDB 1994). Phthalic anhydride is produced by either the oxo process or the Ald-Ox process from ethanol and the oxidation of naphthalene or o-xylene (Peakall 1975). In our process we are using Phthalic Anhydride as a raw material.

Raw Materials:

a. **Phthalic Anhydride**
b. **Ethanol**
c. **H_2SO_4 conc. Catalyst**
d. **Caustic Soda**







The purity of manufactured phthalate esters is reportedly between 99.70% and 99.97% with the main impurities being isophthalic acid, terephthalic acid, and maleic anhydride (Peakall 1975).

The initial charge used consists of phthalic anhydride and ethyl alcohol in the molecular proportion of 1:2, together with 2% by weight of 95% sulphuric acid, aqueous ethyl alcohol of 92% concentration being used. In later charges phthalic anhydride, recycled mono-ethyl phthalate and ethyl alcohol are used in the molecular ratio 0.8:0.2:1.8.

The mixture is refluxed for 6 hours at 95 C. and then the temperature is raised to 120 C. and water and unchanged ethyl alcohol distilled off. Then, while maintaining the temperature at 120 (3., a slow feed of liquid ethyl alcohol is introduced below the surface of the mixture, this operation being continued for 3 hours, the total alcohol introduced being equivalent to about one molecular proportion per two molecular proportions originally used, aqueous alcohol distilling over.

After cooling the crude product is mixed with caustic soda solution of about 20% concentration. On standing the mixture separates into an oily ester layer and an aqueous layer. The ester layer is separated and washed with a quantity of water equal to about one quarter the weight of the phthalic anhydride used initially, and the aqueous extract thus obtained added to the aqueous layer. The washed ester layer, after drying by air blowing at 110 0., is found on analysis to be diethyl phthalate of over **99% purity**. The combined aqueous product is neutralized with sulphuric acid and the methanol present distilled off, after which additional sulphuric acid is added to make the total used equivalent to the caustic soda used, whereupon an oily layer consisting of wet mono-ethyl phthalate containing a little diethyl phthalate form and is separated and dried by air blowing at 110 C. The dry product, which tends to crystallise on standing, is recycled. All the aqueous liquors are distilled for the recovery of ethanol.

The quantity of caustic soda needed being equal to about 5% of the weight of diethyl phthalate made.

In this way, operating with recycling of the monoethyl phthalate, diethy1 phthalate of high purity can be obtained.

References:

https://ntp.niehs.nih.gov/ntp/htdocs/chem_background/exsumpdf/diethyl_phthalate_508.pdf

https://patents.google.com/patent/US2618651A/en

Phthalate esters: Occurrence and biological effects | SpringerLink

List the contributions of each author:

- Author 1 and 2 worked on selection of the chemical.
- Author 2,3,4 worked on the selection of the manufacturing process.
- Author 1,2,3 worked on studying the process in detail, doing its feasibility analysis and other factors.

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