

ABSTRACT

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Title of thesis: Identification of main decomposition products of butane-1,3-diol

Butane-1,3-diol contains three unknown impurities. The relative molecular mass of two of these compounds is 118 and 160 for the last one. The main aim of this work was the identification of these compounds. Due to the low amount of the impurities oxidation by hydrogen peroxide was employed in order to increase their content. As a result of oxidative decomposition two new compounds 3-hydroxybutanal and 4-hydroxybutan-2-one were formed. If the temperature of the oxidation increased to 70 °C acetic acid as a next degradation product was obtained.

The reaction of butane-1,3-diol and 3-hydroxybutanal resulted in a compound of a relative molecular mass 160. Our experiments confirmed that the spectra of our prepared compound and the impurity of butane-1,3-diol were identical. The compound was identified as 1-(4-methyl-1,3-dioxan-2-yl)propan-2-ol using NMR and MS.

The other two compounds of a molecular mass 118 are most likely related compound of the molecular formula $C_6H_{14}O_2$. Their mass spectra were nearly identical and further identification of the structure by means of EI/CI-GC/MS was not successful. The impurities do not arise from the oxidation (or under other stress conditions) and therefore their amount was insufficient for the identification by other techniques (e.g. NMR, IR).