

Benzene structure and electrophilic substitution

Chemistry grades 11-12 (A Level · IB · Class 11-12) · Lab answers

The model answers use the sample data. Your yield and melting point will differ slightly, but the method of calculation and the explanation of temperature control stay the same.

Level: Chemistry grades 11-12 (A Level · IB · Class 11-12) · **Curriculum:** A Level 3.3.10

Question 1 Moles of reactant

$$n = 2.04 \div 136.0 = \mathbf{0.0150 \text{ mol.}}$$

Question 2 Theoretical yield

One mole of ester gives one mole of product: $0.0150 \times 181.0 = \mathbf{2.72 \text{ g.}}$

Question 3 Percentage yield

Percentage yield = $1.63 \div 2.715 \times 100 = \mathbf{60.0 \%}$. Reasons: loss of product in the filtrate and on filter paper, side products such as other isomers or dinitro compounds, and loss during recrystallisation.

Question 4 Temperature control

At higher temperature a second nitro group enters the ring and the acid mixture may oxidise the organic compound, lowering the yield and the purity. The data show a maximum of 9 °C, so the temperature stayed **below 10 °C** as required.

Question 5 Role of sulfuric acid

$\text{HNO}_3 + 2\text{H}_2\text{SO}_4 \rightarrow \text{NO}_2^+ + \text{H}_3\text{O}^+ + 2\text{HSO}_4^-$. Sulfuric acid acts as the **stronger acid that protonates nitric acid**, creating the nitronium ion; it is regenerated, so it is a catalyst.

Question 6 Melting point

A pure solid melts sharply at its literature value; impurities lower and broaden the range. A range of 2 °C ending at 78 °C is **close to the pure value**, so the product is fairly pure but may contain a little of the 2- or 4-isomer.

Question 7 Recrystallisation

Washing removes the remaining acids and soluble impurities; recrystallisation dissolves the solid in hot ethanol and lets pure crystals form on cooling while impurities stay in solution. Improve by using the minimum amount of hot ethanol and cooling slowly in ice, giving **larger, purer crystals**.