

Benzene and Aromatic Compounds

Answer key with worked solutions

A. Structure

1. Structure of benzene.

(a) Kekulé: a hexagon with alternating single and double bonds. Delocalized: a hexagon with a circle inside. (b) Each carbon is **sp²** hybridized, forming three σ bonds (two C–C and one C–H) in a flat ring, with 120° angles. Each carbon has one unhybridized **p orbital** perpendicular to the ring; the six p orbitals overlap side-on all round, so the six π electrons are **delocalized** above and below the ring.

2. Evidence.

Any two: **all C–C bonds are the same length** (139 pm, between 154 and 134 pm); the **enthalpy of hydrogenation** is much less exothermic than for three C=C bonds; benzene **does not decolourize bromine water** and reacts by **substitution** rather than addition.

3. Empirical formula.

In 100 g: C 92.3 g, H 7.7 g.

$$n(\text{C}) = \frac{92.3 \text{ g}}{12.01 \text{ g/mol}} = 7.69 \text{ mol}; n(\text{H}) = \frac{7.7 \text{ g}}{1.008 \text{ g/mol}} = 7.6 \text{ mol}$$

Ratio 7.69 : 7.6 $\approx$ 1 : 1, so the empirical formula is **CH** (and the molecular formula $\text{C}_6\text{H}_6 = 6 \times \text{CH}$).

B. Stability and reactions

4. Delocalization energy.

Expected for three C=C: $3 \times (-120 \text{ kJ/mol}) = -360 \text{ kJ/mol}$. Actual: -208 kJ/mol .

Difference: $-208 - (-360) = \mathbf{152 \text{ kJ/mol}}$. Benzene releases 152 kJ/mol less energy because it starts **152 kJ/mol lower in energy** (more stable) than a structure with three separate double bonds; the extra stability comes from delocalization.

5. Reactions.

(a) **Concentrated HNO₃ + concentrated H₂SO₄**, about **50 °C**: nitrobenzene, C₆H₅NO₂ (+ H₂O). (b) **Br₂** with a **FeBr₃** (or Fe) catalyst: bromobenzene, C₆H₅Br (+ HBr). Both are **electrophilic substitution**.

6. Names.

(a) **methylbenzene** (toluene) (b) **benzoic acid** (c) **chlorobenzene** (d) **phenol**

C. Calculations

7. Bromobenzene.

$$n(\text{C}_6\text{H}_6) = \frac{15.6 \text{ g}}{78.11 \text{ g/mol}} = 0.1997 \text{ mol (1 : 1)}$$
$$m(\text{C}_6\text{H}_5\text{Br}) = 0.1997 \text{ mol} \times 157.01 \text{ g/mol} = \mathbf{31.4 \text{ g}}$$

D. Challenge

8. Nitration of methylbenzene.

$$n(\text{C}_7\text{H}_8) = \frac{9.21 \text{ g}}{92.13 \text{ g/mol}} = 0.09997 \text{ mol (1 : 1)}$$

Theoretical: $0.09997 \text{ mol} \times 137.14 \text{ g/mol} = \mathbf{13.7 \text{ g}}$

Percent yield: $\frac{10.5 \text{ g}}{13.71 \text{ g}} \times 100\% = \mathbf{76.6\%}$