

Molecule Understanding



Problem: Count **methyl groups** number in this molecule: CC1=CC=C(C)C=C1 (**p-Xylene**)

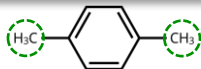


Step-wise Reasoning

- 1 **Identify fragment:** A **methyl group** is $-CH_3$, SMILES=C.
- 2 **Parse molecule SMILES:** CC1=CC=C(C)C=C1 shows two "C" substituents attached to the **aromatic ring**.
- 3 **Match fragment occurrences:** Each "C" outside the **ring** core represents one **methyl**.



Solution: 2



Molecule Optimization



Problem: Optimize the **benzene** to improve the compound's **solubility** property

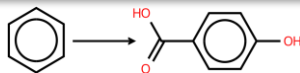


Step-wise Reasoning

- 1 **Structure analysis:** **Benzene** is fully hydrophobic with no **polar** groups.
- 2 **Property analysis:** Negligible **solubility**; no H-bond donors/acceptors.
- 3
 1. Add $-OH$ at C1 to form **phenol**;
 2. Add $-COOH$ at C4 to boost **polarity**;
 3. Confirm **aromaticity** and **valence**.



Solution: O=C(O)c1ccc(O)cc1



Molecule Editing



Problem: Add a **nitro group** and remove the **chlorine substituent** from Clc1ccc(C)cc1

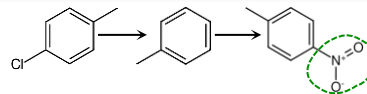


Step-wise Reasoning

- 1 **Functional group analysis:** Locate **Cl** at C-4 and **CH₃** at C-1 on the **benzene**.
- 2 **Delete strategy:** Remove **chlorine substituent** to get Cc1ccccc1 (**toluene**).
- 3 **Add strategy:** Add a **nitro group** at the former Cl site to get CC1=CC=C(C=C1)[N+](=O)[O-] (**4-nitrotoluene**).
- 4 **Feasibility:** Conversion of **toluene** to **4-nitrotoluene** is well-established.



Solution: CC1=CC=C(C=C1)[N+](=O)[O-]



Reaction Prediction



Problem: Predict the **product** from **benzene** and **chloroethane** with **AlCl₃** reagent



Step-wise Reasoning

- 1 **Reactant analysis:** C6H6 (Benzene), CH3CH2Cl (alkyl halide), AlCl3 (catalyst).
- 2 **Identify function group:** Locate **H** at benzene and **CH₃** at chloromethane.
- 3 **Reaction type predict:** **friedel-crafts alkylation**, The electrophile is the methyl carbocation. Benzene attacks the carbocation
- 4 **Product predict:** Ethylbenzene (C6H5CH2CH3)..



Solution: c1ccccc(CC)c1

