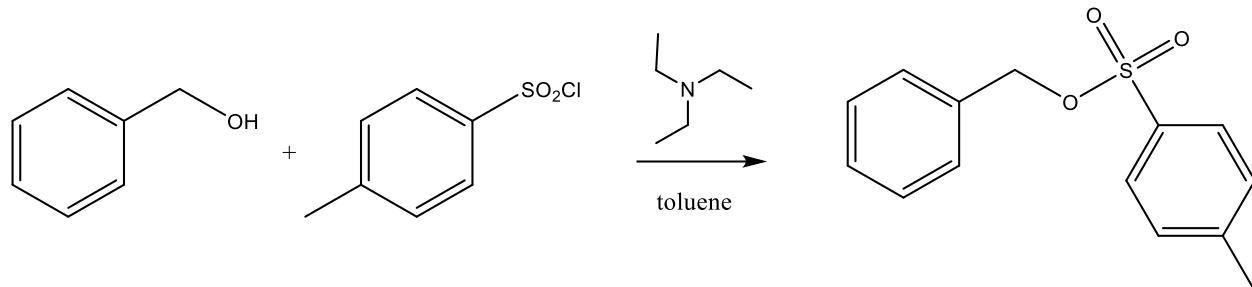


Exercise 3

Calculate the E-factor, atom economy, carbon efficiency, reaction mass efficiency, generalized reaction mass efficiency and solvent intensity for the following reaction.



	MW (kg/kmol)	Mass (kg)	kmol
Benzylalcohol (BnOH)	108	10.8	0.10
TsCl	191	21.9	0.11
Toluene	92.1	500	5.43
Triethylamine	101	15.0	0.15
Sulfonate	262	23.6	0.09

Yield:

$$Y_{BA} = \frac{23.6/262}{10.8/108} = 90.1\%$$

$$Y_{TsCl} = \frac{23.6/262}{21.9/191} = 78.6\%$$

E-Factor:

$$E - factor = \frac{10.8 + 21.9 + 500 + 15 - 23.6}{23.6} = 22.2 \text{ (Assuming no recycling of toluene and unreacted TsCl)}$$

Where *Waste* = All Raw Materials – Valorized Products

Atom economy:

Considered: protecting groups, catalysts used in stoichiometric quantities, acids or bases used for hydrolysis, any chemical that is consumed i.e. incorporated into an intermediate or product

Omitted: solvents, reagents or materials used in catalytic quantities, workup materials

BnOH : Reactant → Consider

TsCl : Reactant → Consider

Toluene : Solvent → Omit

Triethylamine : Catalyst used in stoichiometric quantities → Consider

Sulfonate : Desired final product → Consider as product

$$AE = \frac{262}{108+101+191} = 65.5\%$$

Carbon efficiency:

Do not consider triethylamine and toluene as their carbon atoms are not incorporated into the product

$$CE = \frac{\text{moles of carbon in product}}{\text{Total moles of carbon in reactants}} = \frac{\sum_{\text{product } i} \frac{m_i}{MW_i} \times N_{C_i}}{\sum_{\text{reactant } j} \frac{m_j}{MW_j} \times N_{C_j}}$$

$$CE = \frac{(23.6/262) \cdot 14}{(10.8/108) \cdot 7 + (21.9/191) \cdot 7} = 84.2\%$$

RME :

Takes stoichiometry, yield and atom economy into account.

Not included: waste, toxicity, safety, auxiliaries incl. solvents, workup & purification materials, energy, renewability of raw materials

BnOH : Reactant → Consider

TsCl : Reactant → Consider

Toluene : Solvent → Omit

Triethylamine : Catalyst → Omit

Sulfonate : Desired final product → Consider as product

$$RME = \frac{23.6}{10.8+21.9} = 72.2\%$$

gRME :

Takes yield, atom economy and all materials into account, takes auxiliaries (solvents, catalysts, workup and purification materials) into account.

Not accounted for: toxicity, safety, energy, renewability of raw materials

BnOH : Reactant → Consider

TsCl : Reactant → Consider

Toluene : Solvent → Consider

Triethylamine : Catalyst → Consider

Sulfonate : Desired final product → Consider as product

$$gRME = \frac{23.6}{10.8 + 21.9 + 500 + 15} = 4.3\%$$

Solvent intensity :

$$\text{Solvent intensity} = 500/23.6 = 21.2$$