

Green Chemistry Metrics

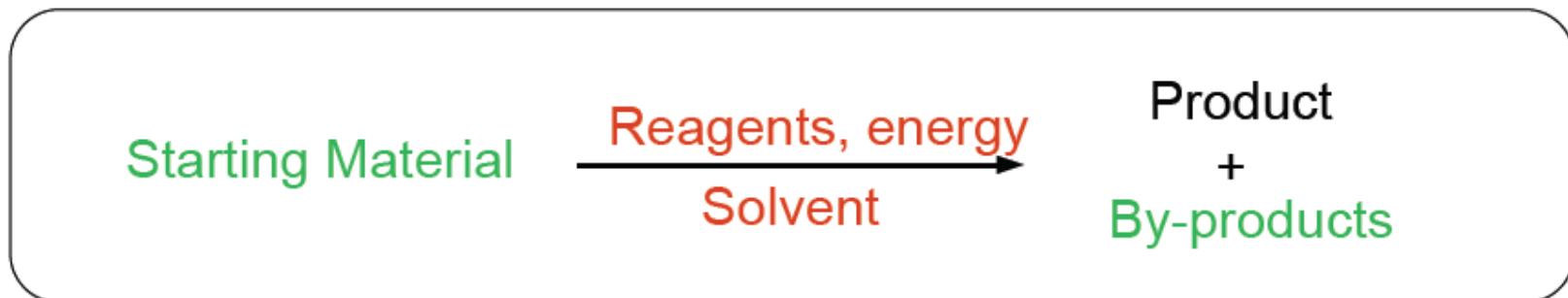


IGSS'09

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*Director of the Marian University
Institute for Green and Sustainable
Science*

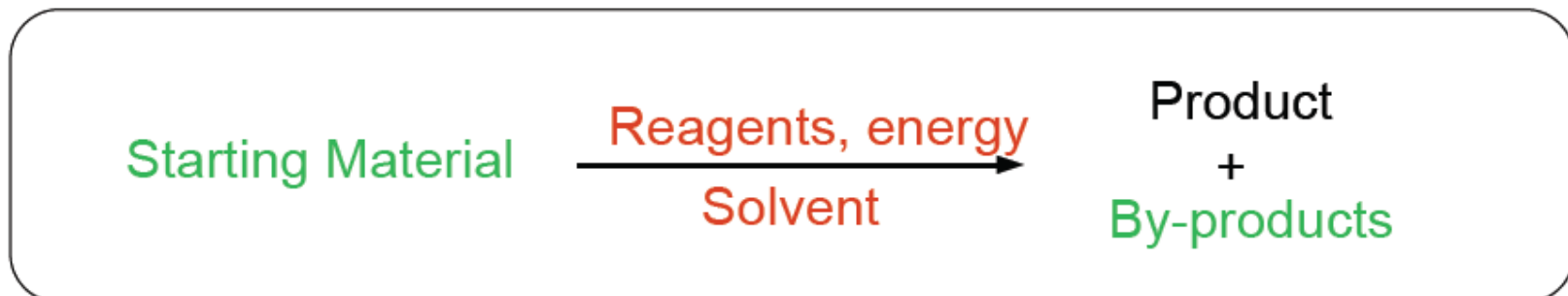
June 29th-July 31st , 2009



review

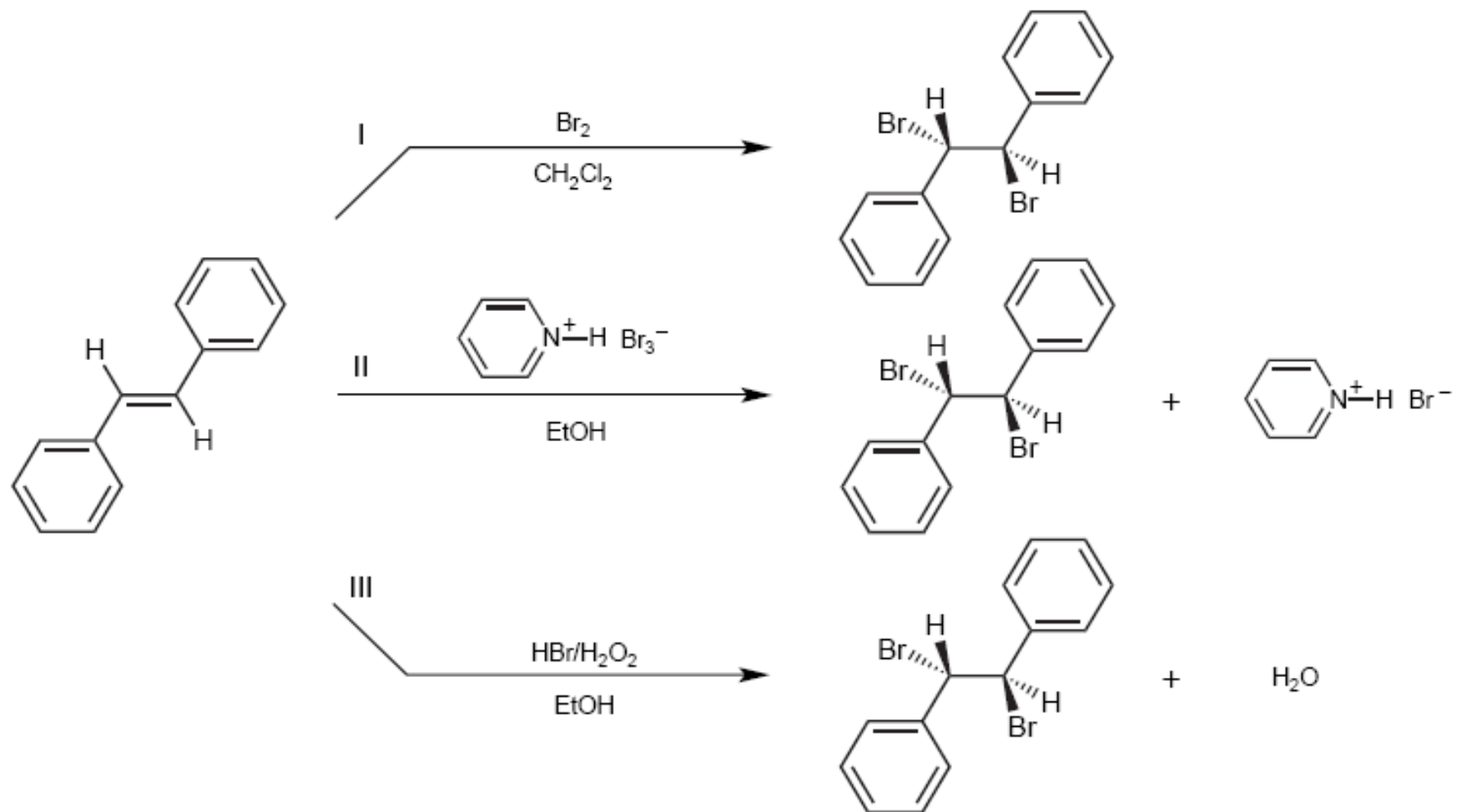
What is atom economy?

What does it measure?



$$\text{Atom economy} = (\text{MW}_{\text{desired product}} / \sum \text{MW}_{\text{reagents}}) \times 100\%$$

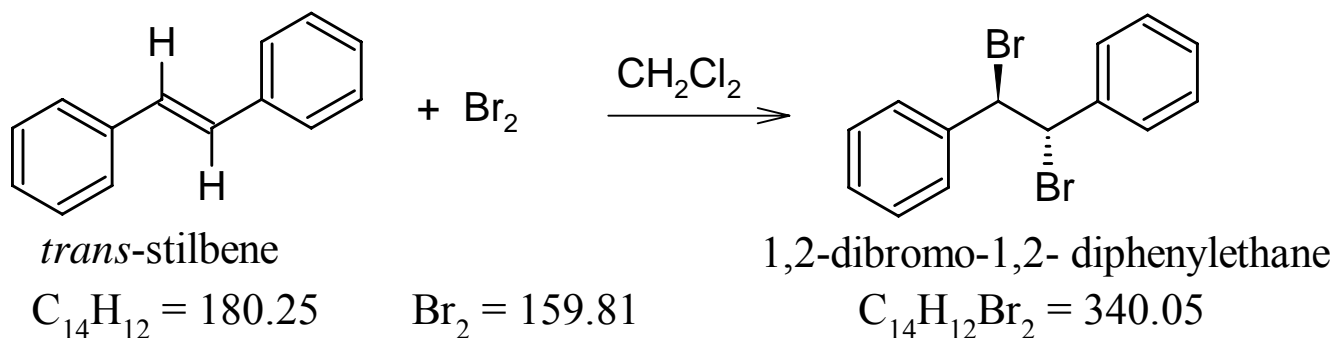
a measure of intrinsic efficiency



McKenzie, L. C.; Huffman, L. M.; Hutchison, J. E. The Evolution of a Green Chemistry Laboratory Experiment: Greener Brominations of Stilbene. *J. Chem. Ed.* **2005**, 82, 306-310

What is the atom economy of this reaction?

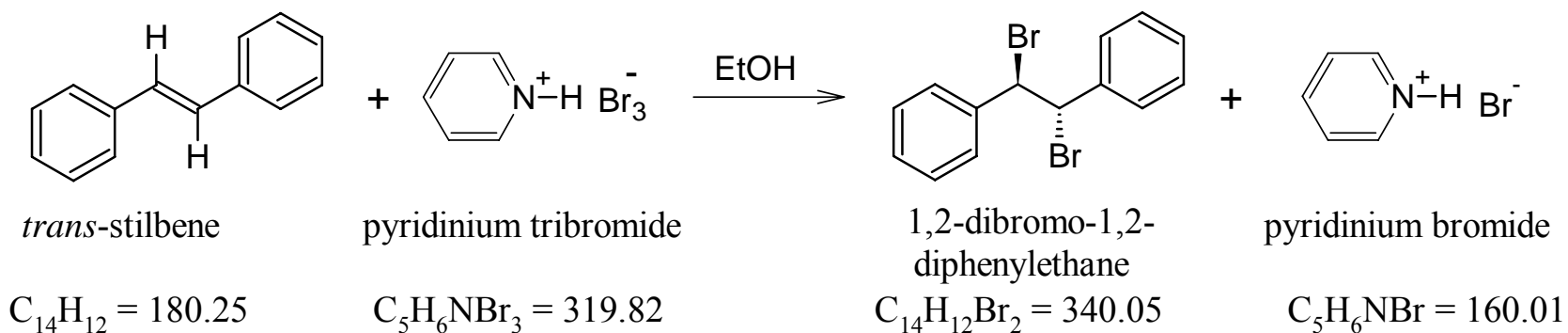
Reaction 1. Traditional Bromination



$$\text{Atom economy} = \left(\frac{\text{MW}_{\text{desired product}}}{\sum \text{MW}_{\text{reagents}}} \right) \times 100\%$$

What is the atom economy of this reaction?

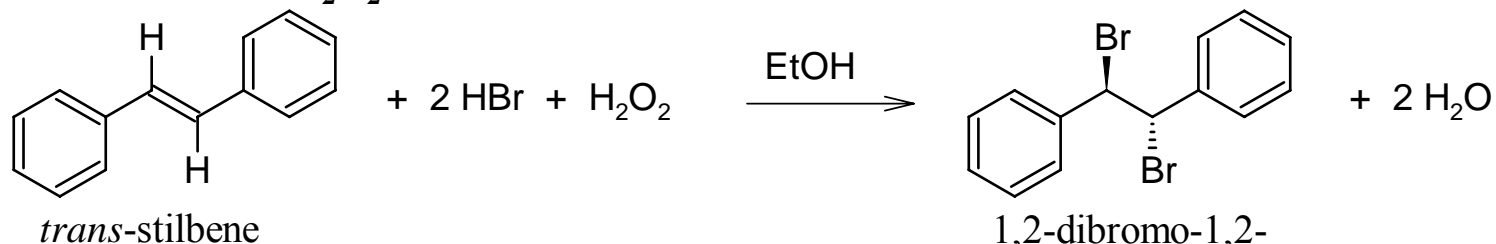
Reaction 2. Pyridinium tribromide



$$\text{Atom economy} = \left(\frac{MW_{\text{desired product}}}{\sum MW_{\text{reagents}}} \right) \times 100\%$$

What is the atom economy of this reaction?

Reaction 3. HBr/H₂O₂



$$\text{C}_{14}\text{H}_{12} = 180.25$$

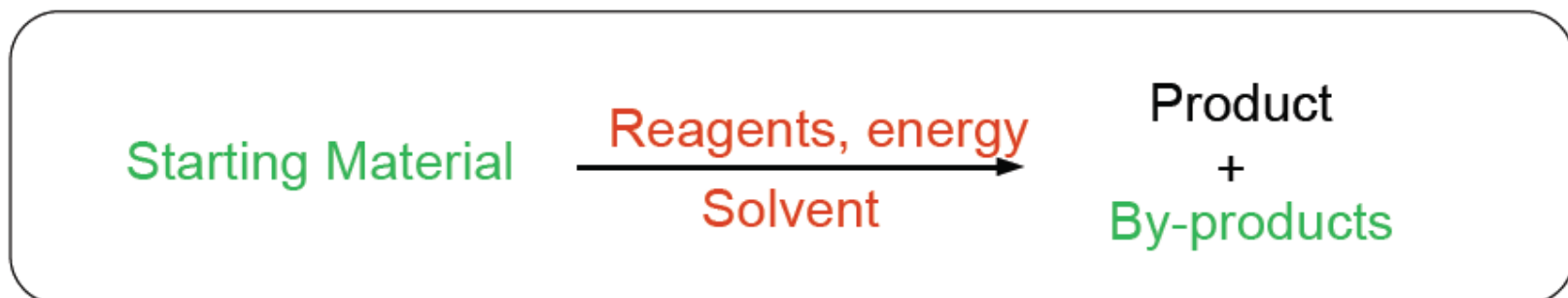
$$\text{HBr} = 80.92$$

$$\text{H}_2\text{O}_2 = 34.02$$

$$\text{C}_{14}\text{H}_{12}\text{Br}_2 = 340.05$$

$$\text{H}_2\text{O} = 18.01$$

$$\text{Atom economy} = \left(\frac{\text{MW}_{\text{desired product}}}{\sum \text{MW}_{\text{reagents}}} \right) \times 100\%$$



A realistic assessment of the efficiency of a reaction must address:
percent yield (a measure of selectivity)
atom economy (a measure of intrinsic efficiency)
deviations from ideal stoichiometry (a measure of the actual efficiency)

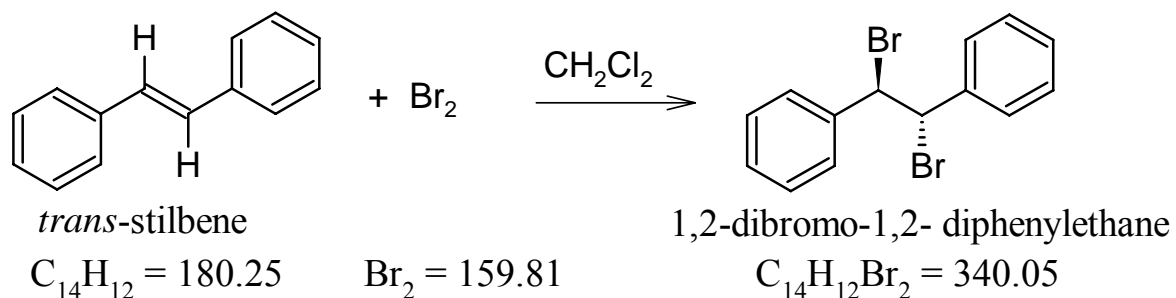
We can easily do that by comparing the mass we put into the reaction to the mass of product we obtain.

If reagents come as aqueous solutions, we ignore the mass of the water.

$$\text{Effective mass yield} = (\text{mass}_{\text{desired product}} / \sum \text{mass}_{\text{reagents}}) \times 100\%$$

What is the effective mass yield of this reaction?

Reaction 1. Traditional Bromination



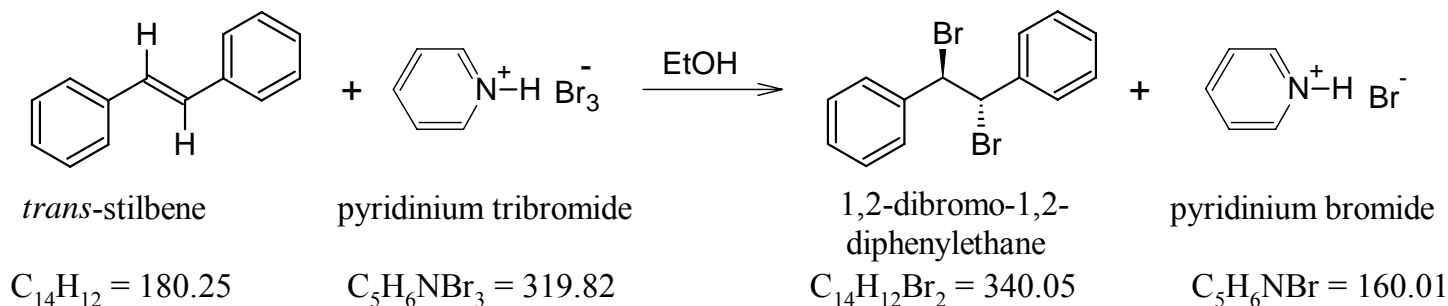
<u>Name</u>	<u>Formula</u> <u>Weight</u>	<u>eq</u>	<u>mmol</u>	<u>wt / vol</u>
<i>trans</i> -stilbene	180.25	1.00	10.0	1.80 g
bromine	159.81	1.05	10.5	1.68 g

Assume 90% yield

$$\text{Effective mass yield} = \left(\frac{\text{mass}_{\text{desired product}}}{\sum \text{mass}_{\text{reagents}}} \right) \times 100\%$$

What is the effective mass yield of this reaction?

Reaction 2. Pyridinium tribromide



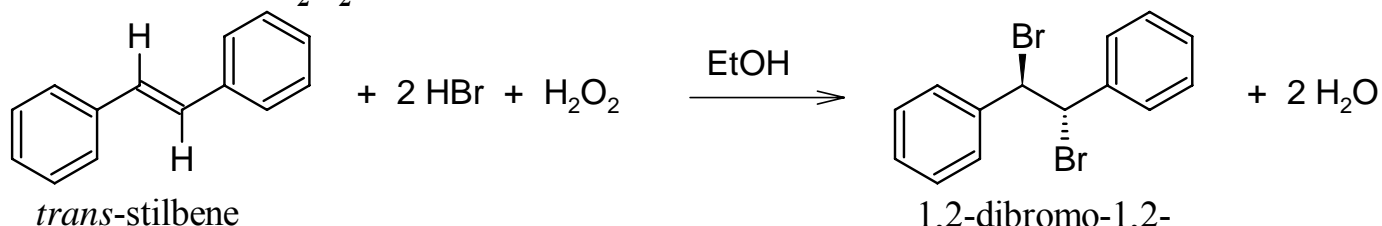
Name	Formula			
	Weight	eq	mmol	wt / vol
<i>trans</i> -stilbene	180.25	1.00	10.0	1.80 g
pyridinium tribromide (90%)	319.82	1.13	11.3	3.61 g

Assume 90% yield

$$\text{Effective mass yield} = \left(\frac{\text{mass}_{\text{desired product}}}{\sum \text{mass}_{\text{reagents}}} \right) \times 100\%$$

What is the effective mass yield of this reaction?

Reaction 3. HBr/H₂O₂



$$C_{14}H_{12} = 180.25$$

$$HBr = 80.92$$

$$H_2O_2 = 34.02$$

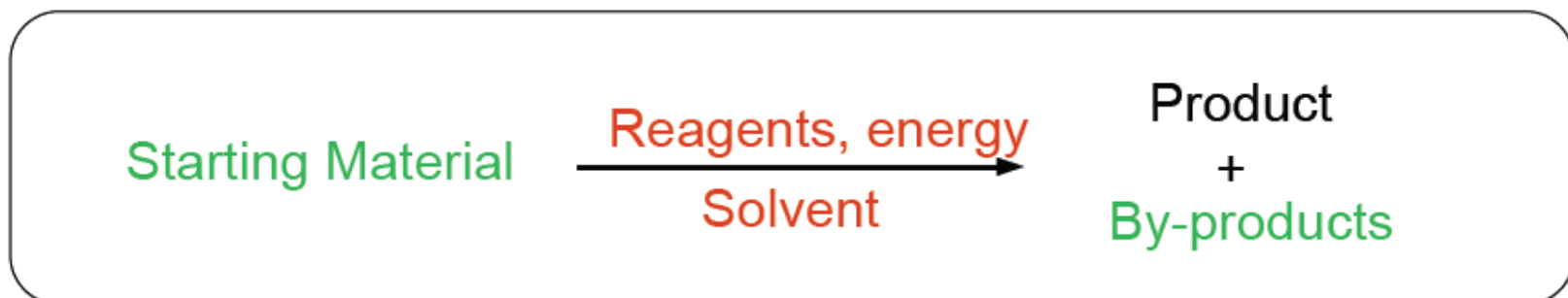
$$C_{14}H_{12}Br_2 = 340.05$$

$$H_2O = 18.01$$

Name	Formula	Weight	density	eq	mmol	wt / vol
<i>trans</i> -stilbene		180.25	--	1.00	10.0	1.80 g
hydrobromic acid 48%		80.92	1.49	2.80	28.0	3.18 mL
hydrogen peroxide 30%		34.02	1.11	2.06	20.6	2.12 mL

Assume 90% yield

$$\text{Effective mass yield} = \left(\frac{\text{mass}_{\text{desired product}}}{\sum \text{mass}_{\text{reagents}}} \right) \times 100\%$$

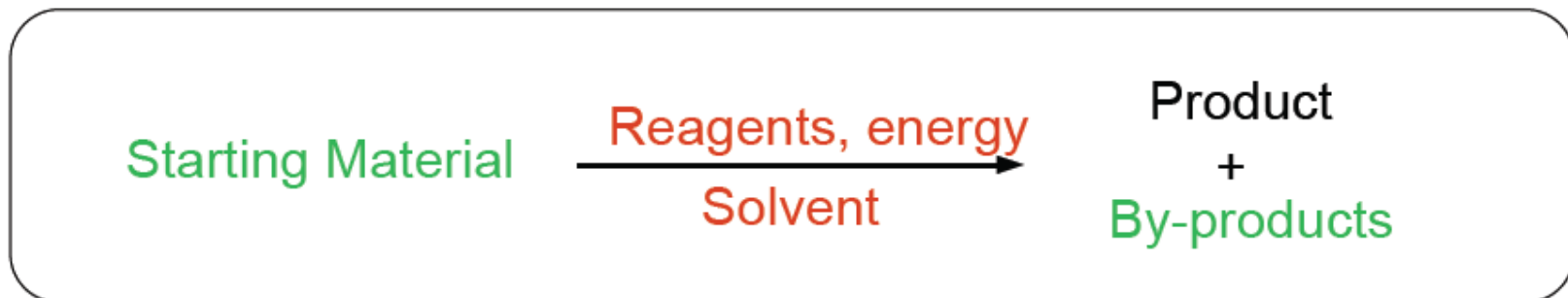


Have we left out any of the mass used?

What about the solvents?

Which do we include?

Which do we exclude?



Add the mass of non-benign solvents to the equation

modify

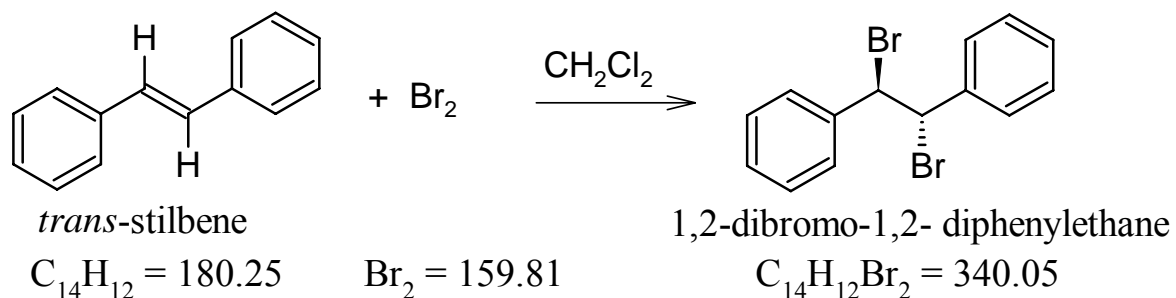
$$\text{Effective mass yield} = (\text{mass}_{\text{desired product}} / \sum \text{mass}_{\text{reagents}}) \times 100\%$$

to

$$\text{Effective mass yield} = (\text{mass}_{\text{desired product}} / \sum \text{mass}_{\text{reagents \& non-benign solvent}}) \times 100\%$$

What is the solvent?

Reaction 1. Traditional Bromination



Name	Formula	Weight	eq	mmol	wt / vol
<i>trans</i> -stilbene		180.25	1.00	10.0	1.80 g
bromine		159.81	1.05	10.5	1.68 g

Is CH_2Cl_2 benign?

What is the mass of CH_2Cl_2 ?

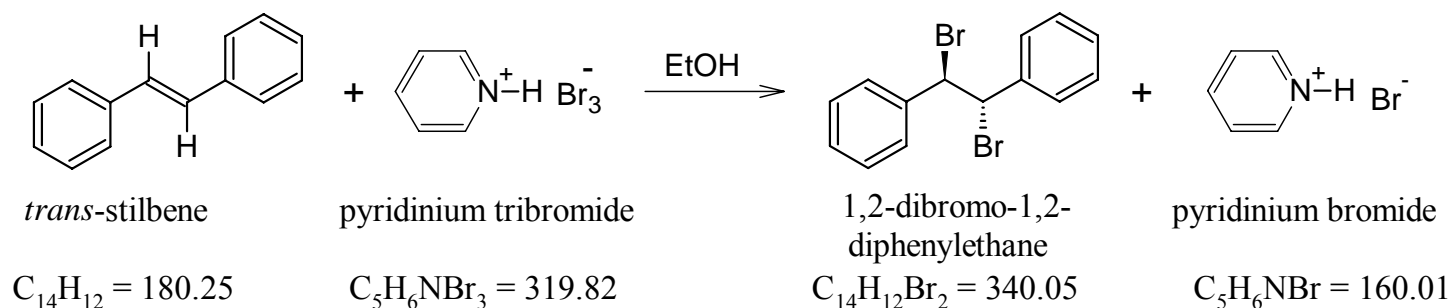
Assume that the concentration of stilbene in CH_2Cl_2 is 0.25 M

Assume 90% yield

$$\text{Effective mass yield} = \left(\frac{\text{mass}_{\text{desired product}}}{\sum \text{mass}_{\text{reagents \& non-benign solvent}}} \right) \times 100\%$$

What is the solvent?

Reaction 2. Pyridinium tribromide



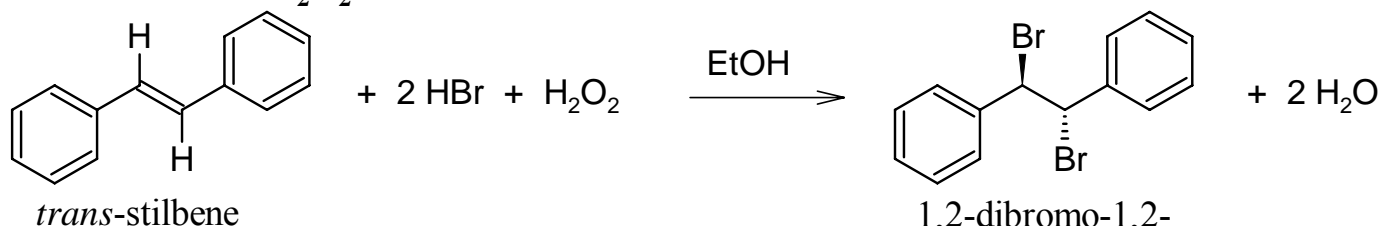
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