## P1.1

$\mathrm{SiO}_{2}+3 \mathrm{C} \rightarrow 2 \mathrm{CO}+\mathrm{SiC}$

## P1.2

$$
\mathrm{C}_{3} \mathrm{H}_{5}\left(\mathrm{NO}_{3}\right)_{3} \rightarrow v_{2} \mathrm{CO}_{2}+v_{3} \mathrm{H}_{2} \mathrm{O}+v_{4} \mathrm{~N}_{2}+v_{5} \mathrm{O}_{2}
$$

From element balances on $\mathrm{N}, \mathrm{C}, \mathrm{H}$, and O , we write 4 equations:

$$
\begin{aligned}
& 3=2 v_{4} \\
& 3=v_{2} \\
& 5=2 v_{3} \\
& 9=2 v_{2}+v_{3}+2 v_{5}
\end{aligned}
$$

Solving, we find
$\mathrm{C}_{3} \mathrm{H}_{5}\left(\mathrm{NO}_{3}\right)_{3} \rightarrow 3 \mathrm{CO}_{2}+\frac{5}{2} \mathrm{H}_{2} \mathrm{O}+\frac{3}{2} \mathrm{~N}_{2}+\frac{1}{4} \mathrm{O}_{2}$

## P1.3

$\left(\mathrm{NH}_{4}\right)_{2} \mathrm{PtCl}_{6} \rightarrow v_{2} \mathrm{Pt}+v_{3} \mathrm{NH}_{4} \mathrm{Cl}+v_{4} \mathrm{~N}_{2}+v_{5} \mathrm{HCl}$
Pt: $v_{2}=1$
$\mathrm{N}: v_{3}+2 v_{4}=2$
H: $4 v_{3}+v_{5}=8$
Cl: $v_{3}+v_{5}=6$
Combine H and Cl balances and solve, than solve N balance:

$$
v_{3}=\frac{2}{3}, v_{5}=5 \frac{1}{3}, v_{4}=\frac{2}{3}
$$

$\left(\mathrm{NH}_{4}\right)_{2} \mathrm{PtCl}_{6} \rightarrow \mathrm{Pt}+\frac{2}{3} \mathrm{NH}_{4} \mathrm{Cl}+\frac{2}{3} \mathrm{~N}_{2}+5 \frac{1}{3} \mathrm{HCl}$

## P1.4

The three balanced equations are

$$
\begin{aligned}
& \mathrm{NaHCO}_{3}+\mathrm{HCl} \rightarrow \mathrm{NaCl}+\mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O} \\
& \mathrm{CaCO}_{3}+2 \mathrm{HCl} \rightarrow \mathrm{CaCl}_{2}+\mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O} \\
& \mathrm{MgCO}_{3}+2 \mathrm{HCl} \rightarrow \mathrm{MgCl}_{2}+\mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O}
\end{aligned}
$$

To calculate the grams HCl neutralized per gram of each compound, we need the molar masses: $84 \mathrm{~g} / \mathrm{gmol}$ for sodium bicarbonate, $100 \mathrm{~g} / \mathrm{gmol}$ for calcium carbonate, and 84 $\mathrm{g} / \mathrm{gmol}$ for magnesium carbonate.
$\mathrm{NaHCO}_{3}: \frac{1 \mathrm{gmol} \mathrm{HCl}}{\mathrm{gmol} \mathrm{NaHCO}_{3}} \times \frac{\mathrm{gmol} \mathrm{NaHCO}}{3}-\frac{36.5 \mathrm{~g} \mathrm{HCl}}{84 \mathrm{~g} \mathrm{NaHCO}_{3}} \times \frac{0.435 \mathrm{~g} \mathrm{HCl}}{\mathrm{gmol} \mathrm{HCl}^{\mathrm{g} \mathrm{NaHCO}} 3}$

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$\mathrm{CaCO}_{3}: \frac{2 \mathrm{gmol} \mathrm{HCl}}{\mathrm{gmol} \mathrm{CaCO}_{3}} \times \frac{\mathrm{gmol} \mathrm{CaCO}_{3}}{100 \mathrm{~g} \mathrm{CaCO}_{3}} \times \frac{36.5 \mathrm{~g} \mathrm{HCl}}{\mathrm{gmol} \mathrm{HCl}}=\frac{0.73 \mathrm{~g} \mathrm{HCl}}{\mathrm{g} \mathrm{CaCO}_{3}}$
$\mathrm{MgCO}_{3}: \frac{2 \mathrm{gmol} \mathrm{HCl}}{\mathrm{gmol} \mathrm{MgCO}_{3}} \times \frac{\mathrm{gmol} \mathrm{MgCO}}{3}$ $\times \frac{36.5 \mathrm{~g} \mathrm{HCl}}{84 \mathrm{~g} \mathrm{MgCO}_{3}}=\frac{0.869 \mathrm{~g} \mathrm{HCl}}{\mathrm{gmol} \mathrm{HCl}}$
$\mathrm{MgCO}_{3}$ has the best neutralizing ability, gram for gram.

## P1.5

Molar mass of urea $\left(\mathrm{NH}_{2}\right)_{2} \mathrm{CO}=2 \times 14+4 \times 1+12+16=60 \mathrm{~g} / \mathrm{gmol}$.
$10 \mathrm{gmol} \times 60 \frac{\mathrm{~g}}{\mathrm{gmol}} \times \frac{1 \mathrm{lb}}{454 \mathrm{~g}}=1.3 \mathrm{lb}$
$10 \mathrm{lbmol} \times 60 \frac{\mathrm{lb}}{\mathrm{lbmol}} \times \frac{454 \mathrm{~g}}{\mathrm{lb}}=272,000 \mathrm{~g}$

## P1.6

Water is required to decompose the urea:

$$
\left(\mathrm{NH}_{2}\right)_{2} \mathrm{CO}+\mathrm{H}_{2} \mathrm{O} \rightarrow 2 \mathrm{NH}_{3}+\mathrm{CO}_{2}
$$

Fractional atom economy $=\frac{2 \mathrm{gmol} \mathrm{NH}_{3} \times(17 \mathrm{~g} / \mathrm{gmol})}{1 \mathrm{gmol} \text { urea } \times(60 \mathrm{~g} / \mathrm{gmol})+1 \mathrm{gmol} \mathrm{H}}{ }_{2} \mathrm{O} \times(18 \mathrm{~g} / \mathrm{gmol}) \quad=0.44$
(with only urea counted in the denominator, fractional atom economy is 0.57 .)

## P1.7

Hexane:
$\mathrm{C}_{6} \mathrm{H}_{14}+9.5 \mathrm{O}_{2} \rightarrow 6 \mathrm{CO}_{2}+7 \mathrm{H}_{2} \mathrm{O}$
$\frac{6 \mathrm{gmol} \mathrm{CO}}{2}$ gmol C $\mathrm{C}_{6} \mathrm{H}_{14} \quad \times \frac{44 \mathrm{~g} \mathrm{CO}_{2} / \mathrm{gmol} \mathrm{CO}_{2}}{86 \mathrm{~g} \mathrm{C}_{6} \mathrm{H}_{14} / \mathrm{gmol} \mathrm{C}_{6} \mathrm{H}_{14}}=3.1 \mathrm{~g} \mathrm{CO}_{2} / \mathrm{g} \mathrm{C}_{6} \mathrm{H}_{14}$
$\frac{7 \mathrm{gmol} \mathrm{H}_{2} \mathrm{O}}{\text { gmol C } \mathrm{C}_{6} \mathrm{H}_{14}} \times \frac{18 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} / \mathrm{gmol} \mathrm{H}_{2} \mathrm{O}}{86 \mathrm{~g} \mathrm{C}_{6} \mathrm{H}_{14} / \mathrm{gmol} \mathrm{C}_{6} \mathrm{H}_{14}}=1.5 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} / \mathrm{g} \mathrm{C}_{6} \mathrm{H}_{14}$

Glucose: $\mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}+6 \mathrm{O}_{2} \rightarrow 6 \mathrm{CO}_{2}+6 \mathrm{H}_{2} \mathrm{O}$
$\frac{6 \mathrm{gmol} \mathrm{CO}}{2}$ gmol C $\mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6} \quad \times \frac{44 \mathrm{~g} \mathrm{CO}_{2} / \mathrm{gmol} \mathrm{CO}_{2}}{180 \mathrm{~g} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6} / \mathrm{gmol} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}}=1.5 \mathrm{~g} \mathrm{CO}_{2} / \mathrm{g} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}$
$\frac{6 \mathrm{gmol} \mathrm{H}}{2} \mathrm{O}-\frac{18 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} / \mathrm{gmol} \mathrm{H}_{2} \mathrm{O}}{\text { gmol C} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}} \times \frac{\mathrm{g} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6} / \mathrm{gmol} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}}{180}=0.6 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} / \mathrm{g} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}$

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## P1.8

$\left(10^{9} \mathrm{lb} \mathrm{NH}_{3}\right)\left(\frac{\mathrm{lbmol} \mathrm{NH}}{3}\right)\left(\frac{\mathrm{lbmol} \mathrm{N}_{2}}{17 \mathrm{lb} \mathrm{NH}_{3}}\right)\left(\frac{28 \mathrm{lb} \mathrm{N}}{2}\right.$ $\left.2 \mathrm{lbmol} \mathrm{NH}_{3}\right)=820$ million lbs $\mathrm{N}_{2}$
$\left(10^{9} \mathrm{lb} \mathrm{NH}_{3}\right)\left(\frac{\mathrm{lbmol} \mathrm{NH}}{3}\right)\left(\frac{3 \mathrm{lbmol} \mathrm{H}}{2}\right)\left(\frac{2 \mathrm{lb} \mathrm{H}_{2}}{17 \mathrm{lb} \mathrm{NH}} 33\right)=180$ million lbs $\mathrm{H}_{2}$

## P1.9

$\mathrm{Cl}_{2}: \frac{\$ 0.016}{\mathrm{gmol}} \times \frac{1 \mathrm{gmol}}{71 \mathrm{~g}} \times \frac{454 \mathrm{~g}}{\mathrm{lb}} \times \frac{2000 \mathrm{lb}}{\text { ton }}=\frac{\$ 205}{\text { ton }}$
$\mathrm{NH}_{3}: \frac{\$ 0.0045}{\mathrm{gmol}} \times \frac{1 \mathrm{gmol}}{17 \mathrm{~g}} \times \frac{454 \mathrm{~g}}{\mathrm{lb}} \times \frac{2000 \mathrm{lb}}{\text { ton }}=\frac{\$ 240}{\text { ton }}$

## P1.10

The conventional process has an atom economy of 0.45 , which means that 0.55 lb reactants are shunted to waste per 0.45 lb of product made. At 300 million lb/yr 4-ADPA production, this amounts 367 million $\mathrm{lb} / \mathrm{yr}$ waste.

The new process, with an atom economy of 0.84 , produces 0.16 lb waste per 0.84 lb product. At 300 million lb/yr 4-ADPA production, this amounts 57 million lb/yr waste, or only $15 \%$ of the waste production of the conventional process.

## P1.11

Molar mass $=2+32+4(16)=98$ tons/tonmol
$\frac{45 \times 10^{6} \text { tons }}{\mathrm{yr}} \times \frac{1 \text { tonmol }}{98 \text { tons }}=4.6 \times 10^{5}$ tonmol $/ \mathrm{yr}$
$\frac{45 \times 10^{6} \text { tons }}{\mathrm{yr}} \times \frac{2000 \mathrm{lb}}{\text { ton }} \times \frac{454 \mathrm{~g}}{\mathrm{lb}}=4.09 \times 10^{13} \mathrm{~g} / \mathrm{yr}$
$\frac{\frac{45 \times 10^{6} \text { tons }}{\mathrm{yr}} \times \frac{2000 \mathrm{lb}}{\text { ton }}}{6 \times 10^{9} \text { people }}=15 \mathrm{lb} /$ person $/ \mathrm{yr}$
$\frac{45 \times 10^{6} \text { tons }}{\mathrm{yr}} \times \frac{\$ 75}{\text { ton }}=\$ 3.4$ billion $/ \mathrm{yr}$

## P1.12

The glucose-to-adipic acid process loses $\$ 5400 /$ day while the benzene to adipic acid process makes $\$ 27,100$. For the glucose process to be competitive, the cost for the glucose needs to drop by $27,100+5400$ or by $\$ 32,500$. The current cost is $\$ 48,500 /$ day, so

[^0]the cost would have to drop to $\$ 16,000$. At $80,850 \mathrm{~kg} /$ day consumption of glucose, this converts to a glucose price of $\$ 0.198 / \mathrm{kg}$.

The glucose-to-catechol process makes $\$ 49,200 /$ day, but the benzene-to-catechol process nets $\$ 89,300$. The difference is $\$ 40,100$. The glucose price would have to drop to $\$ 0.104 / \mathrm{kg}$ to be competitive with benzene.

## P1.13

Some possible explanations: greater number of reactions in pathway, more stringent product purity requirements, less pressure to trim costs by reducing wastes.

## P1.14

$\left(\frac{\$ 2.89}{\text { gal }}\right)\left(\frac{\mathrm{gal}}{8 \mathrm{lb}}\right)=\$ 0.36 / \mathrm{lb}$ : milk is a commodity chemical
$\left(\frac{\$ 1.75}{12 \mathrm{oz}}\right)\left(\frac{16 \mathrm{oz}}{\mathrm{lb}}\right)=\$ 2.33 / \mathrm{lb}$ : at this price, water is a specialty chemical!

## P1.15

$\mathrm{HNO}_{3}+v_{2} \mathrm{CH}_{3} \mathrm{OH} \rightarrow v_{3} \mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}_{2}+v_{4} \mathrm{CO}_{2}+v_{5} \mathrm{H}_{2} \mathrm{O}$
The element balance equations for $\mathrm{N}, \mathrm{C}, \mathrm{H}$ and O are

$$
\begin{aligned}
& 1=v_{3} \\
& v_{2}=3 v_{3}+v_{4} \\
& 1+4 v_{2}=7 v_{3}+2 v_{5} \\
& 3+v_{2}=2 v_{3}+2 v_{4}+v_{5}
\end{aligned}
$$

This is a set of 4 equations in 4 unknowns that we solve by substitution and elimination to find the balanced reaction:

$$
\mathrm{HNO}_{3}+3 \frac{1}{3} \mathrm{CH}_{3} \mathrm{OH} \rightarrow \mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}_{2}+\frac{1}{3} \mathrm{CO}_{2}+3 \frac{2}{3} \mathrm{H}_{2} \mathrm{O}
$$

We want to react ( $54-10 \mathrm{mg} / \mathrm{L}$ ) x 10 L of nitric acid, or 0.44 g . The molar mass of $\mathrm{HNO}_{3}$ is $63 \mathrm{~g} / \mathrm{gmol}$, while that of $\mathrm{CH}_{3} \mathrm{OH}$ is $32 \mathrm{~g} / \mathrm{gmol}$. Therefore:
$0.44 \mathrm{~g} \mathrm{HNO}_{3} \times \frac{\mathrm{gmol} \mathrm{HNO}_{3}}{63 \mathrm{~g} \mathrm{HNO}_{3}} \times \frac{3 \frac{1}{3} \mathrm{gmol} \mathrm{CH}_{3} \mathrm{OH}}{\mathrm{gmol} \mathrm{HNO}_{3}} \times \frac{32 \mathrm{~g} \mathrm{CH}_{3} \mathrm{OH}}{\mathrm{gmol} \mathrm{CH}_{3} \mathrm{OH}}=0.75 \mathrm{~g} \mathrm{CH}_{3} \mathrm{OH}$

## P1.16

The stoichiometrically balanced equation is found by balancing elements:

$$
\mathrm{CF}_{2} \mathrm{Cl}_{2}+2 \mathrm{Na}_{2} \mathrm{C}_{2} \mathrm{O}_{4} \rightarrow 2 \mathrm{NaCl}+2 \mathrm{NaF}+1 \mathrm{C}+4 \mathrm{CO}_{2}
$$

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Grams of sodium oxalate required per gram of Freon-12 destroyed:
$\frac{2 \mathrm{gmol} \mathrm{Na}}{2} \mathrm{C}_{2} \mathrm{O}_{4}\left(\mathrm{gmol} \mathrm{CF}_{2} \mathrm{Cl}_{2} \quad \times \frac{\mathrm{gmol} \mathrm{CF}_{2} \mathrm{Cl}_{2}}{121 \mathrm{~g} \mathrm{CF}_{2} \mathrm{Cl}_{2}} \times \frac{134 \mathrm{~g} \mathrm{Na}_{2} \mathrm{C}_{2} \mathrm{O}_{4}}{\mathrm{gmol} \mathrm{Na}_{2} \mathrm{C}_{2} \mathrm{O}_{4}}=2.21 \mathrm{~g} \mathrm{Na} 2 \mathrm{C}_{2} \mathrm{O}_{4} / \mathrm{g} \mathrm{CF}_{2} \mathrm{Cl}_{2}\right.$
Grams of solid products produced (includes $\mathrm{NaF}, \mathrm{NaCl}$ and C ):

$$
\begin{gathered}
\left(\frac{2 \mathrm{gmol} \mathrm{NaCl}}{\mathrm{gmol} \mathrm{CF}_{2} \mathrm{Cl}_{2}} \times \frac{58.5 \mathrm{~g} \mathrm{NaCl}}{\mathrm{gmol} \mathrm{NaCl}^{m o l}}\right)+\left(\frac{2 \mathrm{gmol} \mathrm{NaF}}{\mathrm{gmol} \mathrm{CF}_{2} \mathrm{Cl}_{2}} \times \frac{42 \mathrm{~g} \mathrm{NaF}}{\mathrm{gmol} \mathrm{NaF}}\right)+\left(\frac{1 \mathrm{gmol} \mathrm{C}}{\mathrm{gmol} \mathrm{CF}_{2} \mathrm{Cl}_{2}} \times \frac{12 \mathrm{~g} \mathrm{C}}{\mathrm{gmol} \mathrm{C}}\right) \\
\times \frac{\mathrm{gmol} \mathrm{CF}_{2} \mathrm{Cl}_{2}}{121 \mathrm{~g} \mathrm{CF}_{2} \mathrm{Cl}_{2}}=1.76 \mathrm{~g} \text { solid products } / \mathrm{g} \mathrm{CF}_{2} \mathrm{Cl}_{2}
\end{gathered}
$$

## P1.17

Ethanol: $\quad \frac{6 \mathrm{gmol} \mathrm{H}}{\mathrm{gmol} \mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}} \times \frac{\mathrm{gmol} \mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}}{46 \mathrm{~g} \mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}} \times \frac{1 \mathrm{~g} \mathrm{H}}{\mathrm{gmol} \mathrm{H}} \times 100 \%=13 \mathrm{wt} \% \mathrm{H}$
Water: $\quad \frac{2 \mathrm{gmol} \mathrm{H}}{\mathrm{gmol} \mathrm{H}} \mathrm{H}_{2} \mathrm{gmol} \mathrm{H} \mathrm{O}-\frac{1 \mathrm{~g} \mathrm{H}}{18 \mathrm{~g} \mathrm{H}_{2} \mathrm{O}} \times \frac{\mathrm{gmol} \mathrm{H}}{} \times 100 \%=11 \mathrm{wt} \% \mathrm{H}$
Glucose: $\quad \frac{12 \mathrm{gmol} \mathrm{H}}{\text { gmol } \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}} \times \frac{\mathrm{gmol} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}}{180 \mathrm{~g} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}} \times \frac{1 \mathrm{~g} \mathrm{H}}{\text { gmol H}} \times 100 \%=6.7 \mathrm{wt} \% \mathrm{H}$

It does seem hard to believe that they achieved $50 \mathrm{wt} \% \mathrm{H}$.

## P1.18

The reactions are balanced by writing element balance equations and solving them simultaneously. The balanced equations are given, along with a calculation of atom economy.

## Hydrogenation:

(a) conventional

$$
\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{COCH}_{3}+\frac{1}{4} \mathrm{NaBH}_{4}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}+\frac{1}{4} \mathrm{NaB}(\mathrm{OH})_{4}
$$

|  | $v_{i}$ | $M_{i}$ | $v_{i} M_{i}$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{COCH}_{3}$ | -1 | 120 | -120 |
| $\mathrm{NaBH}_{4}$ | -0.25 | 38 | -9.5 |
| $\mathrm{H}_{2} \mathrm{O}$ | -1 | 18 | -18 |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}$ | +1 | 122 | 122 |

Atom economy $=122 /(120+9.5+18)=0.83$
(b) catalytic

$$
\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{COCH}_{3}+\mathrm{H}_{2} \rightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}
$$

[^1]Atom economy $=1.0$ !
Oxidation:
(a) conventional
$\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}+\frac{2}{3} \mathrm{CrO}_{3}+\mathrm{H}_{2} \mathrm{SO}_{4} \rightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{COCH}_{3}+\frac{1}{3} \mathrm{Cr}_{2}\left(\mathrm{SO}_{4}\right)_{3}+2 \mathrm{H}_{2} \mathrm{O}$

|  | $v_{i}$ | $\mathbf{M}_{\mathrm{i}}$ | $v_{\mathrm{i}} \mathbf{M}_{\mathrm{i}}$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}$ | -1 | 122 | -122 |
| $\mathrm{CrO}_{3}$ | -0.667 | 100 | -66.7 |
| $\mathrm{H}_{2} \mathrm{SO}_{4}$ | -1 | 98 | -98 |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{COCH}_{3}$ | +1 | 120 | 120 |

Atom economy $=120 /(122+66.7+98)=0.42$
(b) catalytic
$\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}+\mathrm{H}_{2} \mathrm{O}_{2} \rightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{COCH}_{3}+2 \mathrm{H}_{2} \mathrm{O}$
Atom economy $=120 /(122+34)=0.77$
C-C bond formation
(a) conventional
$\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}+\mathrm{Mg}+\mathrm{CO}_{2}+2 \mathrm{HCl} \rightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CHCH}_{3} \mathrm{COOH}+\mathrm{MgCl}_{2}+\mathrm{H}_{2} \mathrm{O}$

|  | $v_{i}$ | $M_{i}$ | $v_{\mathrm{i}} \mathbf{M}_{\mathrm{i}}$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}$ | -1 | 122 | -122 |
| Mg | -1 | 24 | -24 |
| $\mathrm{CO}_{2}$ | -1 | 44 | -44 |
| HCl | -2 | 36.5 | -73 |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CHCH}_{3} \mathrm{COOH}$ | +1 | 150 | 150 |

Atom economy $=150 /(122+24+44+73)=0.57$
(b) catalytic

$$
\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{OH}) \mathrm{CH}_{3}+\mathrm{CO} \rightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CHCH}_{3} \mathrm{COOH}
$$

Atom economy $=1.00$ !

## P1.19

We are told that there may be some water or carbon dioxide made as byproducts in addition to the products shown. To find out if they are, we include them in the reaction,

[^2]solve for stoichiometric coefficients - and check to see whether the coefficients for water and/or carbon dioxide are nonzero. To balance the first reaction, we write
$$
\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{OH}+v_{2} \mathrm{CH}_{3} \mathrm{COCH}_{3} \rightarrow v_{3} \mathrm{C}_{15} \mathrm{H}_{16} \mathrm{O}_{2}+v_{4} \mathrm{CO}_{2}+v_{5} \mathrm{H}_{2} \mathrm{O}
$$

The element balance equations for $\mathrm{C}, \mathrm{O}$ and H are:

$$
\begin{aligned}
& 6+3 v_{2}=15 v_{3}+v_{4} \\
& 6+6 v_{2}=16 v_{3}+2 v_{5} \\
& 1+v_{2}=2 v_{3}+2 v_{4}+v_{5}
\end{aligned}
$$

There are 3 equations and 4 stoichiometric coefficients. Thus, one of them is zero (in other words, that compound is NOT a byproduct.) We find a solution if we set $v_{4}=0$ : $v_{2}$ $=1 / 2, v_{3}=1 / 2, v_{5}=1 / 2$. (There is not a reasonable solution if we assume no water is made.)

We balance the remaining reactions in a similar fashion and find 4 balanced equations

$$
\begin{aligned}
& \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{OH}+\frac{1}{2} \mathrm{CH}_{3} \mathrm{COCH}_{3} \rightarrow \frac{1}{2} \mathrm{C}_{15} \mathrm{H}_{16} \mathrm{O}_{2}+\frac{1}{2} \mathrm{H}_{2} \mathrm{O} \\
& \mathrm{CH}_{4}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{CO}+3 \mathrm{H}_{2} \\
& \mathrm{Cl}_{2}+\mathrm{CO} \rightarrow \mathrm{COCl}_{2} \\
& \mathrm{C}_{15} \mathrm{H}_{16} \mathrm{O}_{2}+\mathrm{COCl}_{2}+2 \mathrm{NaOH} \rightarrow \\
& \quad \frac{1}{50}\left[-\mathrm{OC}_{6} \mathrm{H}_{4} \mathrm{C}\left(\mathrm{CH}_{3}\right)_{2} \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{OCO}-\right]_{\mathrm{n}}+2 \mathrm{NaCl}+2 \mathrm{H}_{2} \mathrm{O}
\end{aligned}
$$

To put together the generation-consumption analysis per mole of polycarbonate, we (a) multiply the $4^{\text {th }}$ reaction by 50 , (b) match phosgene consumption to phosgene generation by multiplying reaction 3 by 50 , (c) match CO consumption to CO generation by multiplying reaction 2 by 50 and (d) match bisphenol A consumption to bisphenol A generation by multiplying reaction 1 by 100 . The result is summarized in table form.

Generation-consumption analysis for production of polycarbonate

|  | R1 | R2 | R3 | R4 | net |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{OH}$ | -100 |  |  |  | -100 |
| $\mathrm{CH}_{3} \mathrm{COCH}_{3}$ | -50 |  |  |  | -50 |
| $\mathrm{C}_{15} \mathrm{H}_{16} \mathrm{O}_{2}$ | 50 |  |  | -50 |  |
| $\mathrm{H}_{2} \mathrm{O}$ | 50 | -50 |  | 100 | +100 |
| $\mathrm{CH}_{4}$ |  | -50 |  |  | -50 |
| CO |  | 50 | -50 |  |  |
| $\mathrm{H}_{2}$ |  | 150 |  |  | +150 |
| $\mathrm{Cl}_{2}$ |  |  | -50 |  | -50 |
| $\mathrm{COCl}_{2}$ |  |  | 50 | -50 |  |
| NaOH |  |  |  | -100 | -100 |
| polycarbonate |  |  |  | 1 | +1 |

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| NaCl |  |  |  | 100 | +100 |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  |  |  |  |

## P1.20

The balanced reactions are found from element balances on $\mathrm{C}, \mathrm{H}, \mathrm{O}$ and N . To determine if water is required as a reactant or product, we postulate that water is a product and then try to balance the equations. If the stoichiometric coefficient for water is zero, it is not a reactant or a product. If it is negative, water is a reactant, if positive, it is a product.

The balanced chemical reactions are

$$
\begin{aligned}
& \mathrm{HCO}_{3}^{-}+\mathrm{NH}_{4}^{+}+\mathrm{C}_{5} \mathrm{H}_{12} \mathrm{O}_{2} \mathrm{~N}_{2} \rightarrow \mathrm{C}_{6} \mathrm{H}_{13} \mathrm{O}_{3} \mathrm{~N}_{3}+2 \mathrm{H}_{2} \mathrm{O} \\
& \mathrm{C}_{6} \mathrm{H}_{13} \mathrm{O}_{3} \mathrm{~N}_{3}+\mathrm{C}_{4} \mathrm{H}_{7} \mathrm{O}_{4} \mathrm{~N} \rightarrow \mathrm{C}_{10} \mathrm{H}_{18} \mathrm{O}_{6} \mathrm{~N}_{4}+\mathrm{H}_{2} \mathrm{O} \\
& \mathrm{C}_{10} \mathrm{H}_{18} \mathrm{O}_{6} \mathrm{~N}_{4} \rightarrow \mathrm{C}_{4} \mathrm{H}_{4} \mathrm{O}_{4}+\mathrm{C}_{6} \mathrm{H}_{14} \mathrm{O}_{2} \mathrm{~N}_{4} \\
& \mathrm{C}_{6} \mathrm{H}_{14} \mathrm{O}_{2} \mathrm{~N}_{4}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{CH}_{4} \mathrm{ON}_{2}+\mathrm{C}_{5} \mathrm{H}_{12} \mathrm{O}_{2} \mathrm{~N}_{2}
\end{aligned}
$$

The generation-consumption table for this set of reactions is:

|  | R1 | R2 | R3 | R4 | net |
| :--- | :--- | :--- | :--- | :--- | :--- |
| bicarbonate | -1 |  |  |  | -1 |
| ammonium | -1 |  |  |  | -1 |
| ornithine | -1 |  |  | +1 | 0 |
| citrulline | +1 | -1 |  |  | 0 |
| water | +2 | +1 |  | -1 | +2 |
| aspartic acid |  | -1 |  |  | -1 |
| arginosuccinate |  | +1 | -1 |  | 0 |
| fumarate |  |  | +1 |  | +1 |
| arginine |  |  | +1 | -1 | 0 |
| urea |  |  |  | +1 | +1 |

The overall reaction is:

$$
\mathrm{HCO}_{3}^{-}+\mathrm{NH}_{4}^{+}+\mathrm{C}_{4} \mathrm{H}_{7} \mathrm{O}_{4} \mathrm{~N} \rightarrow \mathrm{C}_{4} \mathrm{H}_{4} \mathrm{O}_{4}+\mathrm{CH}_{4} \mathrm{ON}_{2}+2 \mathrm{H}_{2} \mathrm{O}
$$

There is net generation of urea, fumarate and water. The urea and water are eliminated in the urine. Fumarate can be used for new amino acid synthesis, or further broken down into $\mathrm{CO}_{2}$ and water.

## P1.21

If all the Fe is incorporated into the nanoparticles, there are $(1.52 / 2)$ or $0.76 \mathrm{mmol} \mathrm{Fe}_{2} \mathrm{O}_{3}$ produced, or, at a molar mass of $160 \mathrm{~g} / \mathrm{gmol}, 0.121 \mathrm{~g}$. The molar mass of $\mathrm{Fe}(\mathrm{CO})_{5}$ is 196 $\mathrm{g} / \mathrm{gmol}$. 1.52 mmol of $\mathrm{Fe}\left(\mathrm{CO}_{5}\right)$ is therefore equal to $(1.52 \times 196 \times 0.001)=0.298 \mathrm{~g}$. Thus, the atom economy is $0.121 /(0.298+1.28+0.34)=0.063$.

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## P1.22

The LeBlanc chemistry is given in Example 1.3. At a sodium carbonate production rate of 1000 ton/day, we complete the following process economy calculations.

| Compound | $v_{i}$ | $\mathbf{M}_{\mathrm{i}}$ | $v_{\mathrm{i}} \mathbf{M}_{\mathrm{i}}$ | tons/day <br> $(\mathrm{SF}=1000 / 106)$ | $\$ /$ ton | $\$ /$ day |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| NaCl | -2 | 58.5 | -117 | -1104 | 95 | $-104,860$ |
| $\mathrm{H}_{2} \mathrm{SO}_{4}$ | -1 | 98 | -98 | -927 | 80 | $-74,160$ |
| HCl | +2 | 36.5 | +73 | +689 |  |  |
| C | -2 | 12 | -24 | -226 |  |  |
| $\mathrm{CO}_{2}$ | +2 | 44 | +88 | +830 |  |  |
| $\mathrm{CaCO}_{3}$ | -1 | 100 | -100 | -943 | 87 | $-82,040$ |
| $\mathrm{Na}_{2} \mathrm{CO}_{3}$ | +1 | 106 | +106 | +1000 | 105 | $+105,000$ |
| CaS | +1 | 72 | +72 | +679 |  |  |
| sum |  |  |  | -2 (close enough to zero) |  | $-156,000$ |

The LeBlanc process looks atrociously bad, at current prices.

## P1.23

The reactions are

$$
\begin{align*}
& \mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}+\frac{1}{2} \mathrm{O}_{2} \rightarrow \mathrm{CH}_{3} \mathrm{CHO}+\mathrm{H}_{2} \mathrm{O}  \tag{R1}\\
& \mathrm{CH}_{3} \mathrm{CHO}+\frac{1}{2} \mathrm{O}_{2} \rightarrow \mathrm{CH}_{3} \mathrm{COOH} \tag{R2}
\end{align*}
$$

Water is the only byproduct.
The generation-consumption analysis is shown in the table.

| Compound | $v_{1}$ | $v_{2}$ | $v_{\text {net }}$ | $\mathrm{M}_{\mathrm{i}}$ | $v_{\mathrm{i}} \mathrm{M}_{\mathrm{i}}$ | kg <br> $(\mathrm{SF}=1 / 60)$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}$ | -1 |  | -1 | 46 | -46 | -0.77 |
| $\mathrm{O}_{2}$ | $-1 / 2$ | $-1 / 2$ | -1 | 32 | -32 | -0.53 |
| $\mathrm{CH}_{3} \mathrm{CHO}$ | +1 | -1 | 0 |  |  |  |
| $\mathrm{H}_{2} \mathrm{O}$ | +1 |  | +1 | 18 | +18 | +0.30 |
| $\mathrm{CH}_{3} \mathrm{COOH}$ |  | +1 | +1 | 60 | +60 | +1.0 |
|  |  |  |  |  |  |  |
| sum |  |  |  |  |  | 0 |

At 0.77 kg ethanol consumed per kg acetic acid generated, and $\$ 0.29 / \mathrm{kg}$ ethanol, the minimum selling price for acetic acid is $0.77(\$ 0.29)=\$ 0.22 / \mathrm{kg}$.

## P1.24

The balanced chemical equations are:

[^3]\[

$$
\begin{align*}
& \mathrm{SiO}_{2}+2 \mathrm{C} \rightarrow \mathrm{Si}+2 \mathrm{CO}  \tag{R1}\\
& \mathrm{Si}+2 \mathrm{Cl}_{2} \rightarrow \mathrm{SiCl}_{4}  \tag{R2}\\
& \mathrm{SiCl}_{4}+2 \mathrm{H}_{2} \rightarrow \mathrm{Si}+4 \mathrm{HCl} \tag{R3}
\end{align*}
$$
\]

| Compound | $v_{1}$ | $v_{2}$ | $v_{3}$ | $v_{\text {net }}$ | $\mathrm{M}_{\mathrm{i}}$ | $v_{\mathrm{i}} \mathrm{M}_{\mathrm{i}}$ | Grams <br> $(\mathrm{SF}=3.57)$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{SiO}_{2}$ | -1 |  |  | -1 | 60 | -60 | -214 |
| C | -2 |  |  | -2 | 12 | -24 | -86 |
| Si | +1 | -1 | +1 | +1 | 28 | +28 | +100 |
| CO | +2 |  |  | +2 | 28 | +56 | +200 |
| $\mathrm{Cl}_{2}$ |  | -2 |  | -2 | 71 | -142 | -507 |
| $\mathrm{SiCl}_{4}$ |  | +1 | -1 |  | 170 |  |  |
| $\mathrm{H}_{2}$ |  |  | -2 | -2 | 2 | -4 | -14 |
| HCl |  |  | +4 | +4 | 36.5 | +146 | +521 |
| sum |  |  |  |  |  |  | 0 |

Reactant and byproduct quantities per 100 g Si produced are shown in the last column.
The atom economy is $28 /(60+24+142+4)=0.12$.

## P1.25

Water is a required byproduct in (R2) and (R3). The balanced reactions are:

$$
\begin{align*}
& \mathrm{C}_{4} \mathrm{H}_{8}+\mathrm{CH}_{2} \mathrm{O} \rightarrow \mathrm{C}_{5} \mathrm{H}_{10} \mathrm{O}  \tag{R1}\\
& \mathrm{C}_{5} \mathrm{H}_{10} \mathrm{O}+\frac{1}{2} \mathrm{O}_{2} \rightarrow \mathrm{C}_{5} \mathrm{H}_{8} \mathrm{O}+\mathrm{H}_{2} \mathrm{O}  \tag{R2}\\
& \mathrm{C}_{5} \mathrm{H}_{10} \mathrm{O}+\mathrm{C}_{5} \mathrm{H}_{8} \mathrm{O} \rightarrow \mathrm{C}_{10} \mathrm{H}_{16} \mathrm{O}+\mathrm{H}_{2} \mathrm{O} \tag{R3}
\end{align*}
$$

We need to multiply (R1) by 2 to avoid making unwanted intermediates. The generationconsumption analysis is:

| Compound | $v_{1}$ | $v_{2}$ | $v_{3}$ | $v_{\text {net }}$ | $\mathbf{M}_{\mathrm{i}}$ | $v_{\mathrm{i}} \mathrm{M}_{\mathrm{i}}$ | Grams <br> $(\mathrm{SF}=1000 / 152)$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C}_{4} \mathrm{H}_{8}$ | -2 |  |  | -2 | 56 | -112 | -737 |
| $\mathrm{CH}_{2} \mathrm{O}$ | -2 |  |  | -2 | 30 | -60 | -395 |
| $\mathrm{C}_{5} \mathrm{H}_{10} \mathrm{O}$ | +2 | -1 | -1 | 0 |  |  |  |
| $\mathrm{O}_{2}$ |  | $-1 / 2$ |  | $-1 / 2$ | 32 | -16 | -105 |
| $\mathrm{C}_{5} \mathrm{H}_{8} \mathrm{O}$ |  | +1 | -1 | 0 |  |  |  |
| $\mathrm{H}_{2} \mathrm{O}$ |  | +1 | +1 | +2 | 18 | +36 | +237 |
| $\mathrm{C}_{10} \mathrm{H}_{10} \mathrm{O}$ |  |  | +1 | +1 | 152 | +152 | +1000 |
|  |  |  |  |  |  |  |  |
| sum |  |  |  |  |  |  | 0 |

Per kg of citral, 0.737 kg butene, 0.395 kg formaldehyde, and 0.105 kg oxygen are required, with 0.237 kg water as the only byproduct.

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## P1.26

The reaction, written with unknown stoichiometric coefficients, is

$$
(\mathrm{CaF}) \mathrm{Ca}_{4}\left(\mathrm{PO}_{4}\right)_{3}+v_{2} \mathrm{H}_{2} \mathrm{SO}_{4}+v_{3} \mathrm{H}_{2} \mathrm{O} \rightarrow v_{4} \mathrm{CaH}_{4}\left(\mathrm{PO}_{4}\right)_{2} \mathrm{H}_{2} \mathrm{O}+v_{5} \mathrm{CaSO}_{4}+v_{6} \mathrm{HF}
$$

We write the element balance equations to find the stoichiomeric coefficients:
Ca: $5=v_{4}+v_{5}$
F: $1=v_{6}$
P: $3=2 v_{4}$
O: $12+4 v_{2}+v_{3}=9 v_{4}+4 v_{5}$
H: $2 v_{2}+2 v_{3}=6 v_{4}+v_{6}$
Balances on F and P are readily solved, followed by the balance on Ca . Finally, H and O balances are solved.

$$
(\mathrm{CaF}) \mathrm{Ca}_{4}\left(\mathrm{PO}_{4}\right)_{3}+3 \frac{1}{2} \mathrm{H}_{2} \mathrm{SO}_{4}+\frac{3}{2} \mathrm{H}_{2} \mathrm{O} \rightarrow \frac{3}{2} \mathrm{CaH}_{4}\left(\mathrm{PO}_{4}\right)_{2} \mathrm{H}_{2} \mathrm{O}+3 \frac{1}{2} \mathrm{CaSO}_{4}+\mathrm{HF}
$$

The process economy calculations are summarized in the table, per ton of monocalcium phosphate.

| Compound | $v_{i}$ | $\mathbf{M}_{\mathrm{i}}$ | $\mathbf{v}_{\mathrm{i}} \mathbf{M}_{\mathrm{i}}$ | Tons <br> $(\mathrm{SF=1/378)}$ | $\$ /$ ton | $\$$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Phosphate rock | -1 | 504 | -504 | -1.33 | 128 | -170 |
| Sulfuric acid | -3.5 | 98 | -343 | -0.91 | 80 | -73 |
| water | -1.5 | 18 | -27 | -0.0714 |  |  |
| Monocalcium phosphate | +1.5 | 252 | +378 | +1 | 320 | +320 |
| Calcium sulfate | +3.5 | 136 | +476 | +1.26 | 320 | +403 |
| Hydrogen fluoride | +1 | 20 | +20 | +0.053 |  |  |
| sum |  |  |  |  |  | +480 |

Required raw materials and byproducts are listed in the "tons" column. The fertilizer is a mix of monocalcium phosphate and calcium sulfate, per ton of mcp, we make 2.26 tons fertilizer. Therefore the net profit is $\$ 480 / 2.26$ tons fertilizer, or $\$ 212 /$ ton.

## P1.27

100 grams of yeast contain
50 g C , or 4.167 gmol C
6.94 g H , or 6.94 gmol H
9.72 g N , or 0.69 gmol N
33.33 g O , or 2.08 gmol O

To normalize to one mole C per mole yeast, we divide all numbers by 4.167. Therefore the "molecular formula" for yeast is $\mathrm{CH}_{1.66} \mathrm{O}_{0.5} \mathrm{~N}_{0.166}$.

[^4]An overall reaction for reaction of glucose, oxygen, and ammonia to yeast, $\mathrm{CO}_{2}$ and water is:

$$
v_{1} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}+v_{2} \mathrm{O}_{2}+v_{3} \mathrm{NH}_{3} \rightarrow v_{4} \mathrm{CH}_{1.66} \mathrm{O}_{0.5} \mathrm{~N}_{0.166}+v_{5} \mathrm{CO}_{2}+v_{6} \mathrm{H}_{2} \mathrm{O}
$$

We know that $3.9 \mathrm{~g} \mathrm{CO}_{2}$ are produced per gram of yeast. The molar mass of $\mathrm{CO}_{2}$ is 44 , and that of "yeast" is $(12+1.66+0.5(16)+0.166(14))=23.98 \mathrm{~g} / \mathrm{gmol}$. Therefore, $3.9(23.98 / 44)$ or $2.1255 \mathrm{gmol} \mathrm{CO}_{2}$ are produced per gmol yeast. We will set $v_{4}=1$ as our basis, and $v_{5}=2.1255$ from these data. Now we can complete the remaining element balances.

C: $6 v_{1}=1+2.1255$
H: $12 v_{1}+3 v_{3}=1.66+2 v_{6}$
O: $6 v_{1}+2 v_{2}=0.5+2(2.1255)+v_{6}$
$\mathrm{N}: v_{3}=0.166$
The balanced reaction is:
$0.521 \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}+2.085 \mathrm{O}_{2}+0.166 \mathrm{NH}_{3} \rightarrow \mathrm{CH}_{1.66} \mathrm{O}_{0.5} \mathrm{~N}_{0.166}+2.1255 \mathrm{CO}_{2}+2.545 \mathrm{H}_{2} \mathrm{O}$
Of the 3.126 gmol C in glucose, 1 gmol is used to make yeast (or about $32 \%$ ) and about $68 \%$ is used to make $\mathrm{CO}_{2}$. (This is probably the best measure of relative utilization of glucose for yeast vs. for $\mathrm{CO}_{2}$.) About $20 \%$ of the mass of carbon containing compounds is yeast, with the remainder as $\mathrm{CO}_{2}$.

## P1.28

A close examination of the first 3 reactions shows that only 2 are independent - if we add reaction 1 and reaction 3 together, we get reaction 2 . Therefore, we need to consider only 2 of these 3 reactions. A generation-consumption table for reactions 1, 3, and 4 is shown (trial 1):

|  | $v_{\mathrm{i} 1}$ | $v_{\mathrm{i} 3}$ | $v_{\mathrm{i} 4}$ | $v_{\text {Innet }}$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{Cu}_{2} \mathrm{~S}$ | -1 |  |  | -1 |
| $\mathrm{Fe}_{2}\left(\mathrm{SO}_{4}\right)_{3}$ | -1 | -1 |  | -2 |
| CuS | +1 | -1 |  | 0 |
| $\mathrm{CuSO}_{4}$ | +1 | +1 | -1 | +1 |
| $\mathrm{FeSO}_{4}$ | +2 | +2 | +1 | +5 |
| S |  | +1 |  | +1 |
| Fe |  |  | -1 | -1 |
| Cu |  |  | +1 | +1 |

To maximize Cu per ton chalcocite, we want to have no net generation of Cu -containing compounds (only metallic Cu ). In other words, we want to find multiplying factors such that

$$
\sum_{k} v_{C u S, k} \chi_{k}=0
$$

and

$$
\sum_{k} v_{\mathrm{CuSO}_{4}, k} \chi_{k}=0
$$

From these restrictions, we find:

$$
\begin{aligned}
& \chi_{1}=\chi_{3} \\
& \chi_{1}+\chi_{3}-\chi_{4}=0
\end{aligned}
$$

We can arbitrarily choose one multiplying factor, so we'll set $\chi_{1}=1=\chi_{3}$, which leaves us with $\chi_{4}=2$. The revised generation-consumption table, along with calculations of mass requirements, is shown.

|  | $v_{\mathrm{i} 1}$ | $v_{\mathrm{i} 3}$ | $v_{\mathrm{i} 4}$ | $v_{\mathrm{I}, \text { net }}$ | $\mathrm{M}_{\mathrm{\imath}}$ | $v_{\mathrm{I}, \text { net }} \mathrm{M}_{\mathrm{i}}$ | Tons <br> $(\mathrm{SF}=1 / 127)$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{Cu}_{2} \mathrm{~S}$ | -1 |  |  | -1 | 159 | -159 | -1.25 |
| $\mathrm{Fe}_{2}\left(\mathrm{SO}_{4}\right)_{3}$ | -1 | -1 |  | -2 | 400 | -800 | -6.3 |
| CuS | +1 | -1 |  | 0 |  |  |  |
| $\mathrm{CuSO}_{4}$ | +1 | +1 | -2 | 0 |  |  |  |
| $\mathrm{FeSO}_{4}$ | +2 | +2 | +2 | +6 | 152 | +912 | +7.18 |
| S |  | +1 |  | +1 | 32 | +32 | +0.25 |
| Fe |  |  | -2 | -2 | 56 | -112 | -0.88 |
| Cu |  |  | +2 | +2 | 63.5 | +127 | +1 |

Per ton of metallic Cu , we need 1.25 tons chalcocite, but also 0.88 tons metallic Fe and an enormous 6.3 tons $\mathrm{Fe}_{2}\left(\mathrm{SO}_{4}\right)_{3} .7 .43$ tons of byproducts are generated.

## P1.29

In the first process, we use lactose to produce glucose with the byproduct galactose. The economic evaluation is summarized in tabular form.

| Compound | $v_{\mathrm{i}}$ | $\mathrm{M}_{\mathrm{i}}$ | $v_{\mathrm{i}} \mathrm{M}_{\mathrm{i}}$ | kg <br> $(\mathrm{SF}=$ <br> $1 / 342)$ | $\$ / \mathrm{kg}$ | $\$$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Lactose | -1 | 342 | -342 | -1 | 0.484 | -0.484 |
| $\mathrm{H}_{2} \mathrm{O}$ | -1 | 18 | -18 | -0.053 |  |  |
| Glucose | +1 | 180 | +180 | +0.526 | 0.60 | +0.316 |
| Galactose | +1 | 180 | +180 | +0.526 |  |  |
| sum |  |  |  |  |  | -0.17 |

We lose 17 cents per kg lactose processed on this deal. If we convert galactose to glucose, we add another $\$ 0.316$ to the last column. With that process modification, we can make about $\$ 0.15 / \mathrm{kg}$ lactose processed.

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## P1.30

Sulfuric acid process
Three reactions

$$
\begin{align*}
& \mathrm{S}+\mathrm{O}_{2} \rightarrow \mathrm{SO}_{2}  \tag{R1}\\
& \mathrm{SO}_{2}+\frac{1}{2} \mathrm{O}_{2} \rightarrow \mathrm{SO}_{3}  \tag{R2}\\
& \mathrm{SO}_{3}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{H}_{2} \mathrm{SO}_{4} \tag{R3}
\end{align*}
$$

These reactions combine easily to an overall reaction of

$$
\mathrm{S}+1.5 \mathrm{O}_{2}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{H}_{2} \mathrm{SO}_{4}
$$

Nitric acid process:
Three balanced reactions are

$$
\begin{align*}
& 2 \mathrm{NH}_{3}+\frac{5}{2} \mathrm{O}_{2} \rightarrow 2 \mathrm{NO}+3 \mathrm{H}_{2} \mathrm{O}  \tag{R1}\\
& \mathrm{NO}+\frac{1}{2} \mathrm{O}_{2} \rightarrow \mathrm{NO}_{2}  \tag{R2}\\
& 3 \mathrm{NO}_{2}+\mathrm{H}_{2} \mathrm{O} \rightarrow 2 \mathrm{HNO}_{3}+\mathrm{NO} \tag{R3}
\end{align*}
$$

The generation-consumption table gives:

| Compound | R1 | R2 | R3 | net |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{NH}_{3}$ | -2 |  |  | -2 |
| $\mathrm{O}_{2}$ | $-5 / 2$ | $-1 / 2$ |  | -3 |
| NO | +2 | -1 | +1 | +2 |
| $\mathrm{H}_{2} \mathrm{O}$ | +3 |  | -1 | +2 |
| $\mathrm{NO}_{2}$ |  | +1 | -3 | -2 |
| $\mathrm{HNO}_{3}$ |  |  | +2 | +2 |
|  |  |  |  |  |

This doesn't satisfy the restrictions on the solution, e.g., we have NO generated and $\mathrm{NO}_{2}$ consumed, which are not allowed. To have no net generation or consumption of these two intermediates, we find multiplying factors such that

$$
\begin{aligned}
& 2 \chi_{1}-\chi_{2}+\chi_{3}=0 \\
& \chi_{2}-3 \chi_{3}=0
\end{aligned}
$$

Choosing arbitrarily $\chi_{1}=1$, we find the solution is $\chi_{2}=3$ and $\chi_{3}=1$. The new generationconsumption table is

| Compound | R1 | R2 | R3 | net |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{NH}_{3}$ | -2 |  |  | -2 |
| $\mathrm{O}_{2}$ | $-5 / 2$ | $-3 / 2$ |  | -4 |

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| NO | +2 | -3 | +1 |  |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{H}_{2} \mathrm{O}$ | +3 |  | -1 | +2 |
| $\mathrm{NO}_{2}$ |  | +3 | -3 |  |
| $\mathrm{HNO}_{3}$ |  |  | +2 | +2 |
|  |  |  |  |  |

## For an overall reaction of

$\mathrm{NH}_{3}+2 \mathrm{O}_{2} \rightarrow \mathrm{HNO}_{3}+\mathrm{H}_{2} \mathrm{O}$
The difference in value of nitric vs sulfuric acid is likely due to the difference in cost of ammonia vs sulfur. Sulfur is a byproduct of oil refining (desulfurization) and is available in very large quantities. Ammonia, on the other hand, is synthesized from nitrogen and methane in a high pressure, high temperature process.

## P1.31

Analysis of the process economy is summarized in the table. A multiplying factor of 3 was use in reaction R 2 to eliminate generation/consumption of intermediates.

| compound | $v_{1}$ | $v_{2}$ | $v_{\text {net }}$ | $\mathrm{M}_{\mathrm{i}}$ | $v_{\text {net }} \mathrm{M}_{\mathrm{i}}$ | Lb <br> $(\mathrm{SF}=1 / 918)$ | $\$ / \mathrm{lb}$ | $\$$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Glycerol stearate | -1 |  | -1 | 890 | -890 | -0.97 | 1.00 | -0.97 |
| $\mathrm{H}_{2} \mathrm{O}$ | -3 | +3 |  | 18 |  |  |  |  |
| Stearic acid | +3 | -3 |  | 284 |  |  |  |  |
| glycerol | +1 |  | +1 | 92 | +92 | 0.100 | 1.10 | +0.11 |
| NaOH |  | -3 | -3 | 40 | -120 | -0.13 | 0.50 | -0.065 |
| Sodium stearate |  | +3 | +3 | 306 | +918 | +1 | x | x |

To just break even, we need $x-0.97+0.11-0.065=0$, or $x=\$ 0.925 / \mathrm{lb}$ soap. I found soap available in 18 lb quantities for about $\$ 2 /$ pound on an internet site. You'll spend about $\$ 2$ for a 4 oz bar of soap at the drugstore.

## P1.32

This problem is designed to encourage students to learn how to find and to use KirkOthmer and other reference books.

## P1.33

Reaction pathway 1:
The balanced chemical reactions are

$$
\begin{align*}
& \mathrm{C}_{4} \mathrm{H}_{6}+2 \mathrm{HCN} \rightarrow \mathrm{C}_{6} \mathrm{H}_{8} \mathrm{~N}_{2}  \tag{R1}\\
& \mathrm{C}_{6} \mathrm{H}_{8} \mathrm{~N}_{2}+4 \mathrm{H}_{2} \rightarrow \mathrm{C}_{6} \mathrm{H}_{16} \mathrm{~N}_{2} \tag{R2}
\end{align*}
$$

The process economy evaluation, at $116,000 \mathrm{lb}$ /day, is summarized in a table.

| compound | $v_{1}$ | $v_{2}$ | $v_{\text {net }}$ | $\mathrm{M}_{\mathrm{i}}$ | $v_{\text {net }} \mathrm{M}_{\mathrm{i}}$ | Lb <br> $(\mathrm{SF}=1000)$ | $\$ / \mathrm{lb}$ | $\$$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C}_{4} \mathrm{H}_{6}$ | -1 |  | -1 | 54 | -54 | -54000 | 0.21 | $-11,340$ |

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