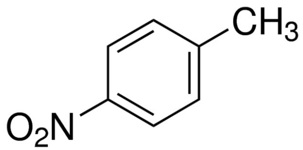
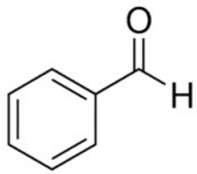
Chemical Reaction Safety Workshop

Solution to Exercises

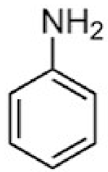
Ex 1. Solution:



$C_7H_7NO_2$



C_7H_6O



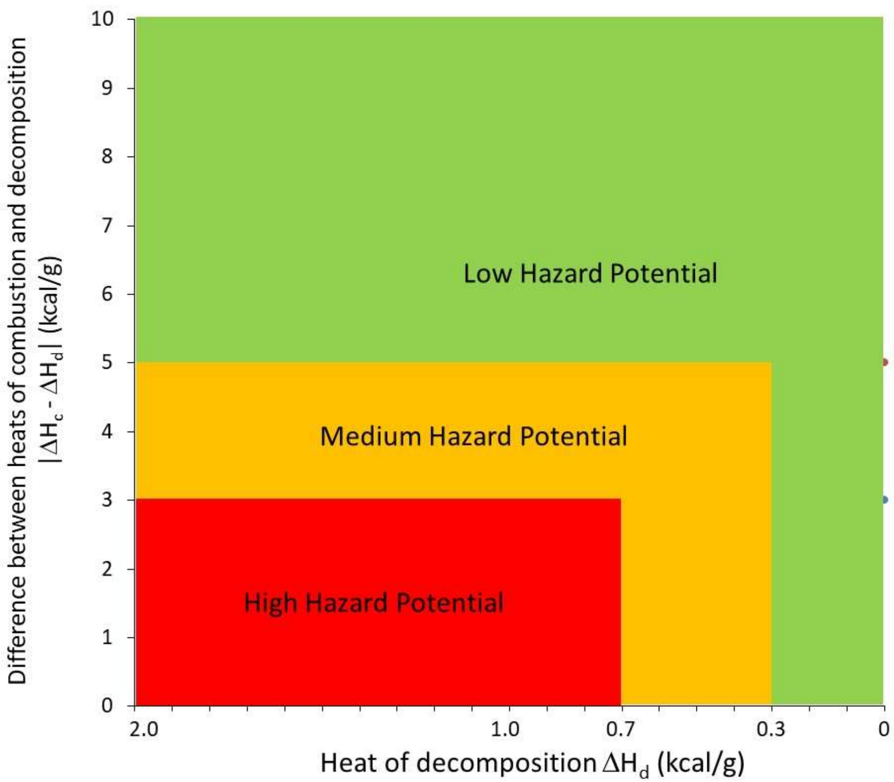
$C_6H_5NH_2$

	nitrotoluene	Benzaldehyde	Aniline
MW (g/mol)	137	106	93
ΔHc (J/g)	2.62E+04	33254.71698	3.48E+04
ΔHc (kcal/g)	6.26	7.95	8.32
ΔHd (J/g)	**-3520**	**-1100**	**-820**
ΔHd (kcal/g)	**-0.8**	**-0.3**	**-0.2**
OB	**-181.0**	**-241.5**	**-266.7**
γ	**57.0**	**5.2**	**2.6**
Hc - Hd	**5.4**	**7.7**	**8.1**

$$OB = \frac{-1600(2x + (y/2) - z)}{MW}$$

$$\gamma_{criterion} = \frac{10Q^2(MW)}{N}$$

Ex 1. Solution:



Criterion	Energy Hazard Potential		
	Low	**Medium**	**High**
1	$\Delta H_d > -1255 J/g$	$-2929 < \Delta H_d < -1255 J/g$	$\Delta H_d < -2929 J/g$
2	*Refer to relationship between heats of combustion and decomposition*		
3	OB < -240 OB > 160	-240 < OB < -120 80 < OB < 160	-120 < OB < 80
4	$\gamma < 30$	$30 < \gamma < 110$	$\gamma > 110$

Ex 2. Solution:

A. Desired Reaction

- Is Reactant A likely to decompose under normal process conditions?
- What is the adiabatic temperature rise (ΔT_{ad}) of the primary reaction?

$$\Delta T_{ad} = \frac{Q_r}{c_p} = \frac{250}{1.7} = 147\ \text{K}$$

- What is the final temperature?

Final temperature = process temperature + ΔTad = 80+147 = 227 °C

- Can the decomposition temperature be triggered by the desired reaction?
- If so, what will be the final temperature?

$$\Delta T_{ad} = \frac{Q_r}{c_p} = \frac{960}{1.7} = 565\ \text{K} \qquad \Rightarrow T_{final} = 227 + 565 = 792\ °\text{C}$$

Ex 2. Solution:

Calculate $E_a = \frac{R ln(q_1/q_2)}{\frac{1}{T_2} - \frac{1}{T_1}}$ Using

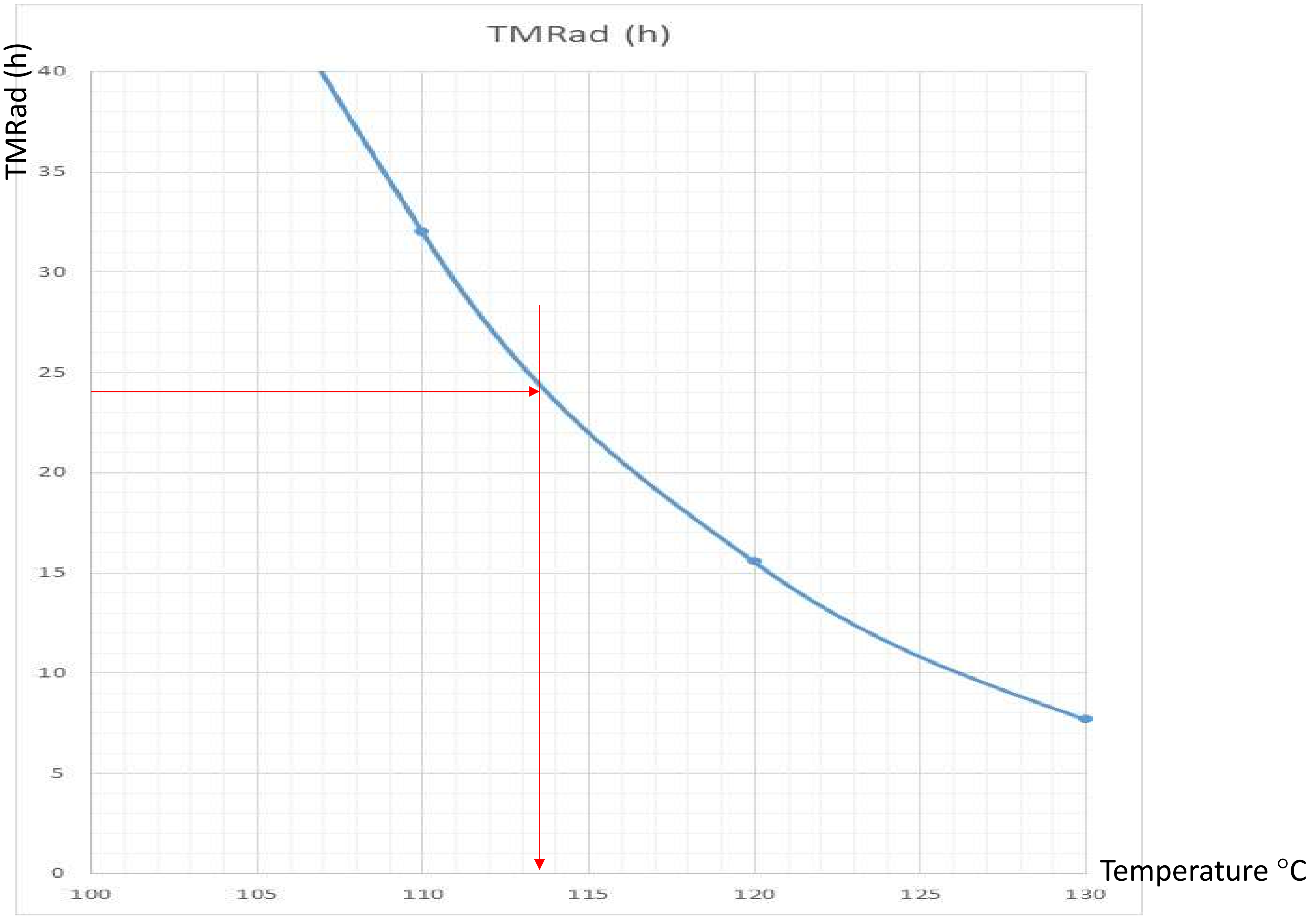
T (°C)	190	200	210	220
q_{max} (W/kg)	40	70	120	190

$$E_a = \frac{(8.314) ln(40/70)}{\frac{1}{473} - \frac{1}{463}}$$ ≈ 100 kJ/mol

$$TMR_{ad} = \frac{C_p R T^2}{q E_a}$$

T (°C)	q_{max} (W/kg)	T (K)	TMRad (s)	TMRad (h)
220	190	493	180.8003	0.050222
210	120	483	274.7717	0.076325
200	70	473	451.7344	0.125482
190	40	463	757.4621	0.210406
180	22.5	453	1289.059	0.358072
170	12.4	443	2236.89	0.621358
160	6.6	433	4015.049	1.115291

as a rule of thumb, we usually assume that a 10 ℃ increase in temperature will result in doubling of the rate of a reaction


TMRad (h)
TMRad (h)
40
35
30
25
20
15
10
5
0
100
105
110
115
120
125
130
Temperature °C

T_{D24} = ? °C

Ex 3. Solution:

- What is the minimum temperature difference between the cooling medium and reaction mixture required for stable reactor performance?

$$T_{crit} = \frac{E}{2R}\left(1 \pm \sqrt{1 - \frac{4RT_0}{E}}\right)$$

E	100000	J/mol
R	8.314	J/K.mol
To	15	288K

Coolant temperature T_0 = 15 °C

Tcrit	11732.6573K
	295.247399K

minimum temperature difference required for stable reactor performance

$$\Delta T_{crit} = T - T_0 \geq \frac{RT_{crit}^2}{E}$$

RTcrit2/E	7.24739916
T	295.247399K
	22.2473992degC

Ex 3. Solution:

- What is the maximum temperature of the cooling medium that will allow for a stable reactor if the required process temperature is 80 °C?

$$\Delta T_{crit} = T - T_0 \geq \frac{R T_{crit}^2}{E}$$

↔

$$T_{crit} = \frac{E}{2R}\left(1 \pm \sqrt{1 - \frac{4RT_0}{E}}\right)$$

To = 69.6 °C= 342.6 K coolant temperature