Contents

1 Alcanes

1.1 Butane [A.1]

$$H-C-C-C-C-H$$

1.2 Cyclohexane [A.2]

1.3 Hexane [A.3]
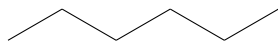
1.4 Isobutane [A.4]

2 Alcohols

2.1 Butanol [??]

$$\begin{array}{ccccccc}
 & H & & H & & H & & H \\
 & | & & | & & | & & | \\
H- & C & - & C & - & C & - & C & -OH \\
 & | & & | & & | & & | \\
 & H & & H & & H & & H
\end{array}$$
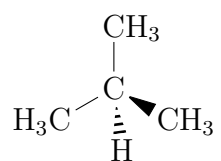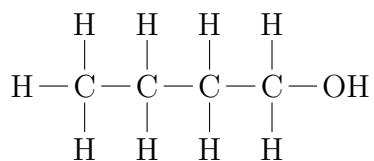
2.2 Cyclohexanol [??]
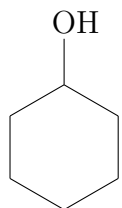
2.3 Hexanol [??]
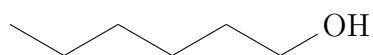
2.4 Isobutanol [??]

2.5 Methanol [??]
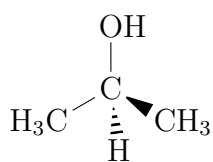
$$\begin{array}{c}
H \\
| \\
H-C-OH \\
| \\
H
\end{array}$$
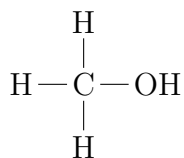
2.6 Mannitol [??]
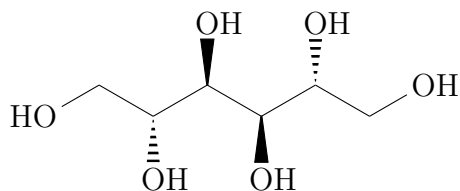
3 Carboxylic Acids

3.1 Acetic Acid [B.1]

3.2 Acrylic Acid [B.2]
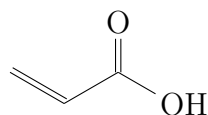
3.3 Benzoic Acid [B.3]
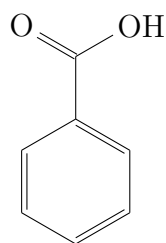
3.4 Fumaric Acid [B.4]
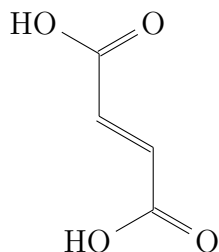
3.5 Maleic Acid [B.5]

3.6 Oleic Acid [B.6]

4 Polymers

4.1 Poly(Bisphenol A Carbonate) [C.1]

$$\left[\rule{0pt}{40pt} \right]_n$$

4.2 Polyurethane [C.2]
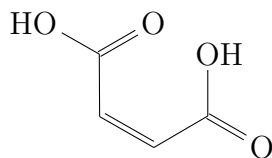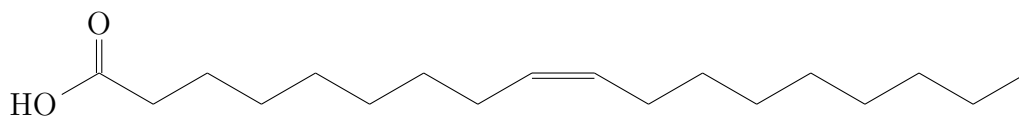
5 Mass Spectrometry

5.1 1-Propanol [D.1]

$$\text{H}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underline{\text{O}}-\text{H} \;+\; e^- \longrightarrow \text{H}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\overset{\bullet\,+}{\underline{\text{O}}}-\text{H} \;+\; 2\,e^-$$

Propan-1-ol $\qquad\qquad\qquad$ m/z = 60

$$\text{H}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underline{\text{O}}^+ \quad + \;\; \text{H}\cdot$$

m/z = 59 $\qquad\qquad$ Δm = 1

$$^+\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underline{\text{O}}-\text{H} \longrightarrow \underset{\text{H}}{\overset{\text{H}}{\diagdown}}\text{C}=\overset{+}{\underline{\text{O}}}-\text{H}$$

m/z = 31

$$\text{H}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}\cdot$$
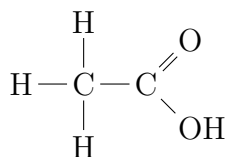
Δm = 29

$$\text{H}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}-\overset{\overset{\text{H}}{|}}{\overset{+}{\text{C}}}-\underset{\underset{\text{H}}{|}}{\overset{\overset{\text{H}}{|}}{\text{C}}}\cdot \quad + \quad \text{H}_2\text{O}$$

m/z = 42 $\qquad\qquad$ Δm = 18

5.2 Ethylbenzene [D.2]

Ethylbenzol

m/z = 106

m/z = 77   + · C$_2$H$_5$

Δm = 29

m/z = 91   + · CH$_3$

Δm = 15

m/z = 51   + C$_2$H$_2$

Δm = 26

m/z = 65   + C$_2$H$_2$

Δm = 26
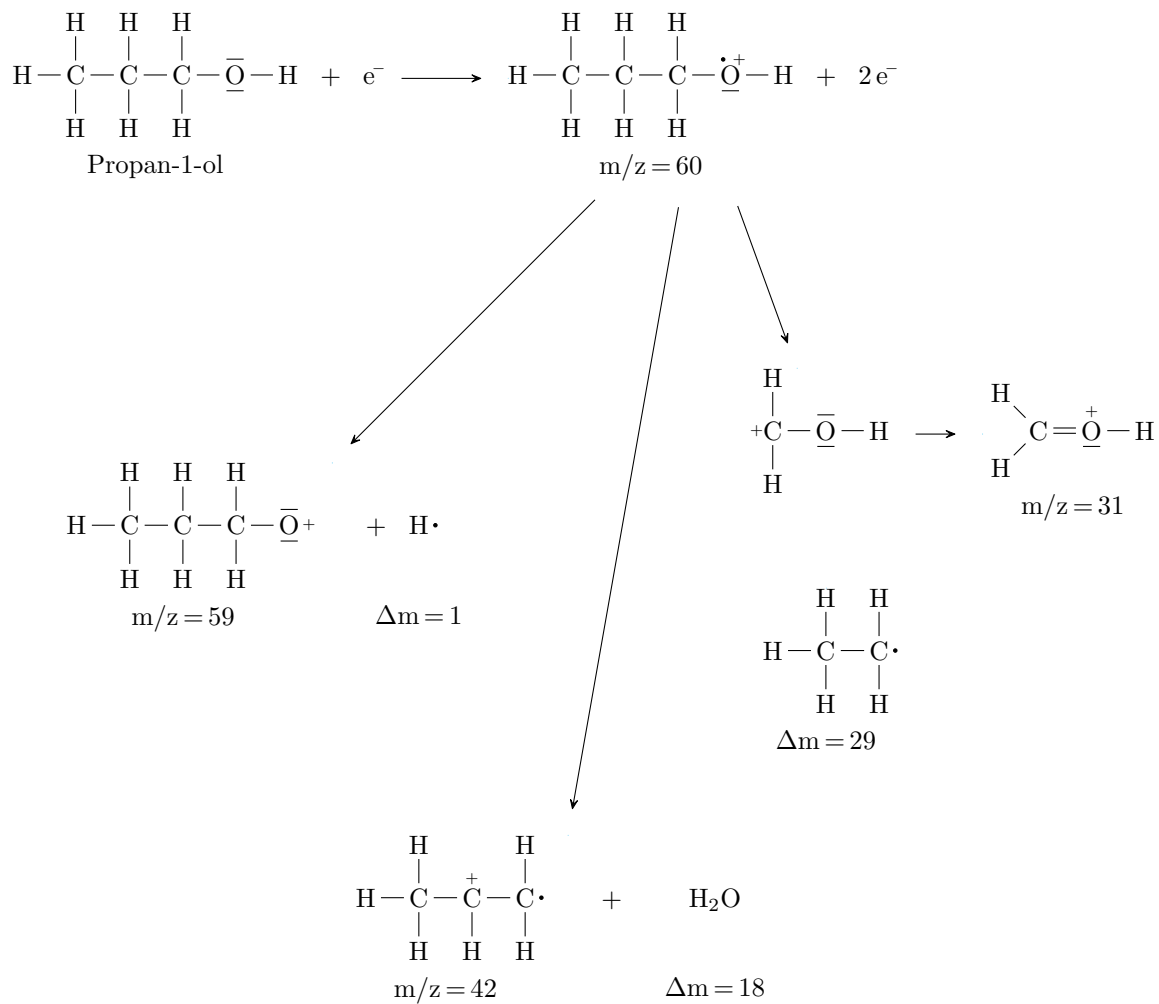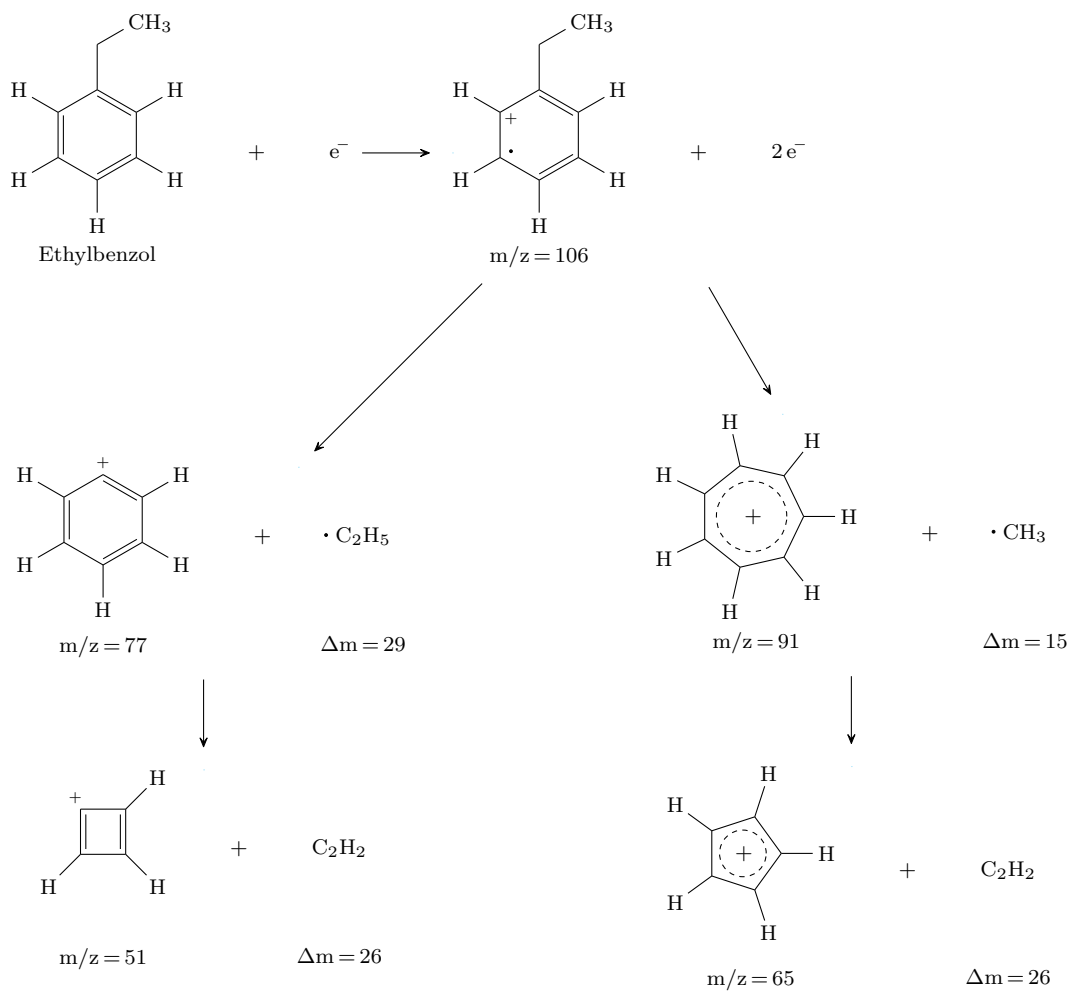
Appendix

Appendix list

A Alcanes

A.1 Butane

```
\chemfig{H-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-
   C(-[2]H)(-[-2]H)-H}
```

A.2 Cyclohexane

```
\chemfig{*6(------)}
```

A.3 Hexane

```
\chemfig[angle increment=30]{-[1]-[-1]-[1]-[-1]-[1]}
```

A.4 Isobutane

```
\chemfig[angle increment=30]{H_3C-[1]C(<:[-2.75]H)(-[3]CH_3)
   <[-1]CH_3}
```

B Carboxylic Acids

B.1 Acetic Acid

```
\chemfig[]{H-C(-[2]H)(-[-2]H)-C(-[-1]OH)=[1]O}
```

B.2 Acrylic Acid

```
\chemfig[angle increment=30]{=^[-1]-[1](-[-1]OH)=[3,0.8]O}
```

B.3 Benzoic Acid

```
\chemfig{*6(-=-=(-(=[3.333]O)(-[0.666]OH))-=)}
```

B.4 Fumaric Acid

```
\chemfig{HO-[:-30](-[-2](=_[:-30](-[-2](=[:-30]O)(-[4.666]HO))
   ))=[:30]O}
```

B.5 Maleic Acid

```
\chemfig[baseline=(b.base)]{HO-[-0.66](=[0.666]O)(*6(-@{b
   }=-(-[2]OH)(=[-0.666]O)))}
```

B.6 Oleic Acid

```
\chemfig[]
{HO-[0.666](=[2,0.8]O)
   -[-0.666]-[0.666]-[-0.666]-[0.666]-[-0.666]-[0.666]-[-0.666]

-[0.666]=_
   -[-0.666]-[0.666]-[-0.666]-[0.666]-[-0.666]-[0.666]-[-0.666]

-[0.666]}
```

C polymers

C.1 Poly(Bisphenol A Carbonate)

```
\chemfig
{\phantom{-}@{op}(-[0.666](=[2]O)(-[-0.666]O
   (-[0.666]*6(=-=(-[0.666](-[2.666]H_3C)(-[1.333]CH_3)
   (-[-0.666](*6(=-=(-[-0.666]O(-[
    0.666]@{cl}))-=-))))-=-)))))}
     \polymerdelim[open xshift = 7.5pt, close xshift = 3.5pt,
        height = 45pt, depth = 10pt, delimiters={[]}, indice =
        \!\!n]{op}{cl}
```

C.2 Polyurethane

```
\chemfig[]
{-[@{op,.5}]C(=[2]O)-N(-[-2]H)-*6(-=-(-C(-*6(=-=(-N(-[-2]H)-C
   (=[2]O)-O-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-O-[@{cl,0.5}])
   -=-))(-[
    2]H)
    (-[-2]H))=-=)}
     \polymerdelim[height = 20pt, depth = 20pt, delimiters
        ={[]}, indice = \!\!n]{op}{cl}
```

D Mass Spectrometry

D.1 1-Propanol

```
\schemestart
\chemname{\chemfig{H-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-\
    charge{90:1pt=\|,-90:1pt=\|}{O}-H}}{Propan-1-ol}
\+
\chemfig{\charge{45=$\scriptscriptstyle{-}$}{e}}
\arrow(.mid east--.mid west)
\chemname
{\chemfig{H-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-\charge
    {115:1pt=\.,-90:1pt=\|,60:1pt=$\scriptscriptstyle{+}$}{O}-H}}
{m/z\,=\,60}
\+
\chemfig{2\,\charge{45=$\scriptscriptstyle{-}$}{e}}
\arrow(@c2--n1)[-70,1.5]
\chemname{\chemfig{\charge{180:1pt=$\scriptscriptstyle{+}$}{C}(-[2]H)
    (-[-2]H)-\charge{90:1pt=\|,-90:1pt=\|}{O}-H}}{\phant
\arrow(.mid east--.mid west)[0,0.7]
\chemnameinit{}
\chemname{\chemfig{C(-[3]H)(-[-3]H)=\charge{90:2pt=$\scriptscriptstyle{+}
    $,-90:1pt=\|}{O}-H}}{m/z\,=\,31}
\chemnameinit{}
\arrow(@c2--n2)[-100,5]
\chemname{\chemfig{H-C(-[2]H)(-[-2]H)-\charge{90:2pt=$\scriptscriptstyle
    {+}$}{C}(-[-2]H)-\charge{0:1pt=\.}{C}(-[2]H)(-[-2]H)}}
{m/z\,=\,42}\qquad
\+\qquad
\chemname{\chemfig{H_2O}}{$\Delta$m\,=\,18}
\chemnameinit{}
\arrow(@c2--n4)[225,3]
\chemname
{\chemfig{H-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-C(-[2]H)(-[-2]H)-\charge
    {90:1pt=\|,-90:1pt=\|,0:2pt=$\scriptscriptstyle{+}$}{O}}}
{m/z\,=\,59}\qquad
\+
\chemname{\chemfig{\charge{0:1pt=\.}{H}}}{$\Delta$m\,=\,1}
\arrow(@n1--nn1)[-90,0.45,white]
\chemname{\chemfig{H-C(-[2]H)(-[-2]H)-\charge{0:1pt=\.}{C}(-[2]H)(-[-2]H)
    }}{$\Delta$m\,=\,29}
\schemestop
```

D.2 Ethylbenzene

```
\schemestart
    \chemname{\chemfig{*6((-H)-(-H)=(-H)-(-H)=(-[2](-[0.666]
        CH_3))-(-H)=(-H))}}{Ethylbenzol} \qquad
    \+ \qquad
    \chemfig{\charge{45=$\scriptscriptstyle{-}$}{e}}
    \arrow(.mid east--.mid west)
    \chemname{\chemfig{*6(\charge{30:3pt=\.}{}(-H)-(-H)=(-H)
        -(-H)=(-[2](-[0.666]CH_3))-\charge{-30:3pt=$\
        scriptscriptstyle{+}$}{}(-H
)-(-H))}}{m/z\,=\,106} \qquad
    \+ \qquad
    \chemfig{2\,\charge{45=$\scriptscriptstyle{-}$}{e}}
    \arrow(@c2--n1)[-60,1.5]
    \chemname{\chemfig{**[0,360,dash pattern=on 2pt off 2pt
        ]7(\charge{25:18.5pt=\+}{}(-H)-(-H)-(-H)-(-H)-(-H)-(-H)
        -(-H)-(-H))}}{m/z\,=\,91}
    \qquad \+ \qquad % +
    \chemname{\chemfig{\charge{180:2pt=\.}{C}H_3}}{$\Delta$m
        \,=\,15}
    \arrow(@n1--m2)[-90,1]
    \chemname{\chemfig{**[0,360,dash pattern=on 2pt off 2pt
        ]5(\charge{35:13pt=\+}{}(-H)-(-H)-(-H)-(-H)-(-H)-(-H)
        -(-H)-)}}{m/z\,=\,65}
    \qquad \+ \qquad
    \chemname{\chemfig{C_2H_2}}{$\Delta$m\,=\,26}
    \arrow(@c2--n4)[225,2.5]
    \chemname{\chemfig{*6((-H)-(-H)=(-H)-(-H)=\charge{90:3pt=$
        \scriptscriptstyle{+}$}{}-(-H)=(-H))}}{m/z\,=\,77}
    \qquad \+ \qquad
    \chemname{\chemfig{\charge{180:2pt=\.}{C}_2H_5}}{$\Delta$m
        \,=\,29}
    \arrow(@n4--m2)[-90,1]
    \chemname{\chemfig{*4((-H)-(-H)=(-H)-\charge{115:3pt=$\
        scriptscriptstyle{+}$}{}=)}}{m/z\,=\,51}
    \qquad \+ \qquad
    \chemname{\chemfig{C_2H_2}}{$\Delta$m\,=\,26}
\schemestop
```