SODAR (Sum Of Double bonds And Rings)

\[
SODAR = \frac{(2x \#C's) + 2 - (\#monovalents) + (\#trivalents)}{2}
\]

What do we do with a SODAR calculation? Look at an example.

\[
C_7H_6O
\]

\[
SODAR = \frac{(2 \times 7) + 2 - 6 + 0}{2} = \frac{10}{2} = 5
\]

This means that any structure that we draw must have a total of five pi bonds and/or rings.

*Any time you see a SODAR of four or greater, start thinking about benzene rings.*

*One ring plus three pi bonds gives a SODAR of four immediately!*

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**Compound Name:** UNKNOWN #1B

**Analytical Data:**
- 70.58 %C
- 5.92 %H

**Molecular Formula:**
- C8H8O2

**Notes:**
- assuming benzene
- aldehyde
- ether?

**Molecular Mass:**
- 136.15

\[
\begin{align*}
70.58 \text{ C} & \quad 5.92 \text{ H} & \quad 23.5 \text{ O} \\
\div 12 & \quad \div 1 & \quad \div 16 \\
5.88 & \quad 5.92 & \quad 1.47 \\
4 & \quad 4 & \quad 1 \\
\text{C8H8O2} & \quad \times 2 \\
\end{align*}
\]
Disubst. benzene - possibilities:

IR Spectrum
NMR Spectrum
Show Integration

Compound Name:
UNKNOWN #18

Analytical Data:
70.58 %C
5.92 %H

Molecular Formula:
C_{8}H_{8}O_{2}

Molecular Mass:
136.15

5.88 : 5.92 : 1.47
4 : 4 : 1
C_{4}H_{4}O \times 2
C_{8}H_{8}O_{2}

SODAR = 5

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Useful Numbers to Remember

$\sim 1$ ppm $CH_3's$  $CH_2, CH$

$\sim 5$ ppm alkenes

$\sim 7$ ppm benzenes/ aromatics

$\sim 9$ ppm aldehyde $\overset{O}{C}=O$

$\sim 12$ ppm carboxylic acid $\overset{O}{C}-OHH$

attached to electronegative atom (O, N, X) $\rightarrow$ downfield

attached to π bond (C=C, C=O) $\rightarrow$ downfield but not as much.