# SODAR (Sum Of Double bonds And Rings)

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

H's, halogens N

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

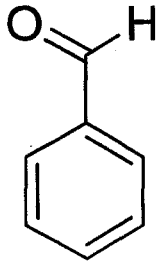
$C_7H_6O$

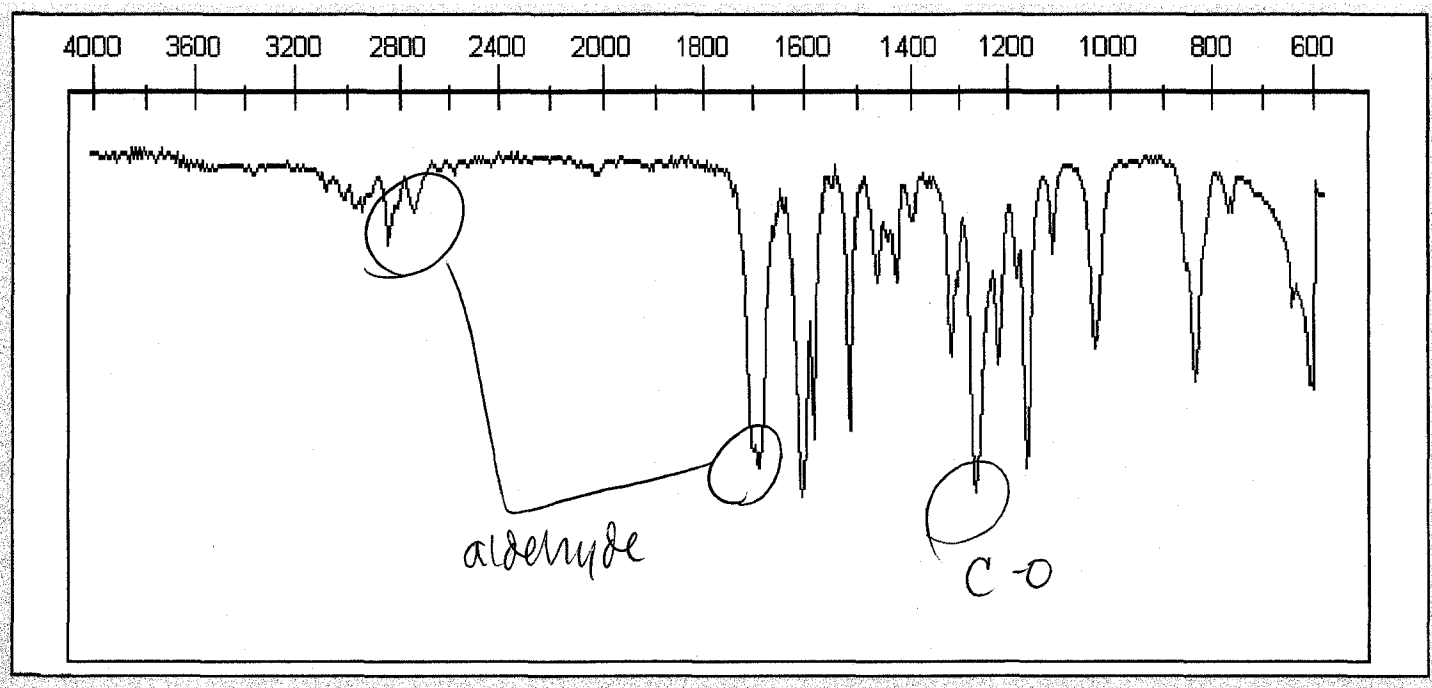
$$SODAR = \frac{(2x7) + 2 - 6 + 0}{2} = \frac{10}{2} = 5$$

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!***






IR Spectrum

NMR Spectrum

Show Integration

Compound Name:
UNKNOWN #18

Analytical Data:
70.58 %C 5.92 %H

Molecular Formula:
---

~~Molecular Mass~~:
136.15

Notes

- assuming benzene
- aldehyde
- ether?

Show Structure | Add Label | Remove Labels

70.58 C ÷ 12 : 5.92 H ÷ 1 : 23.5 O ÷ 16

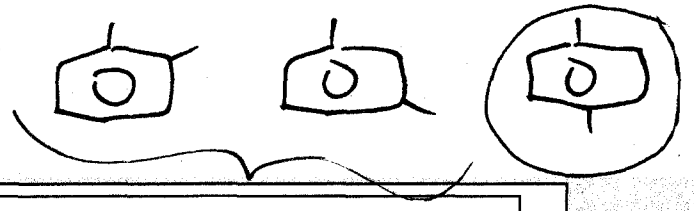
5.88 : 5.92 : 1.47

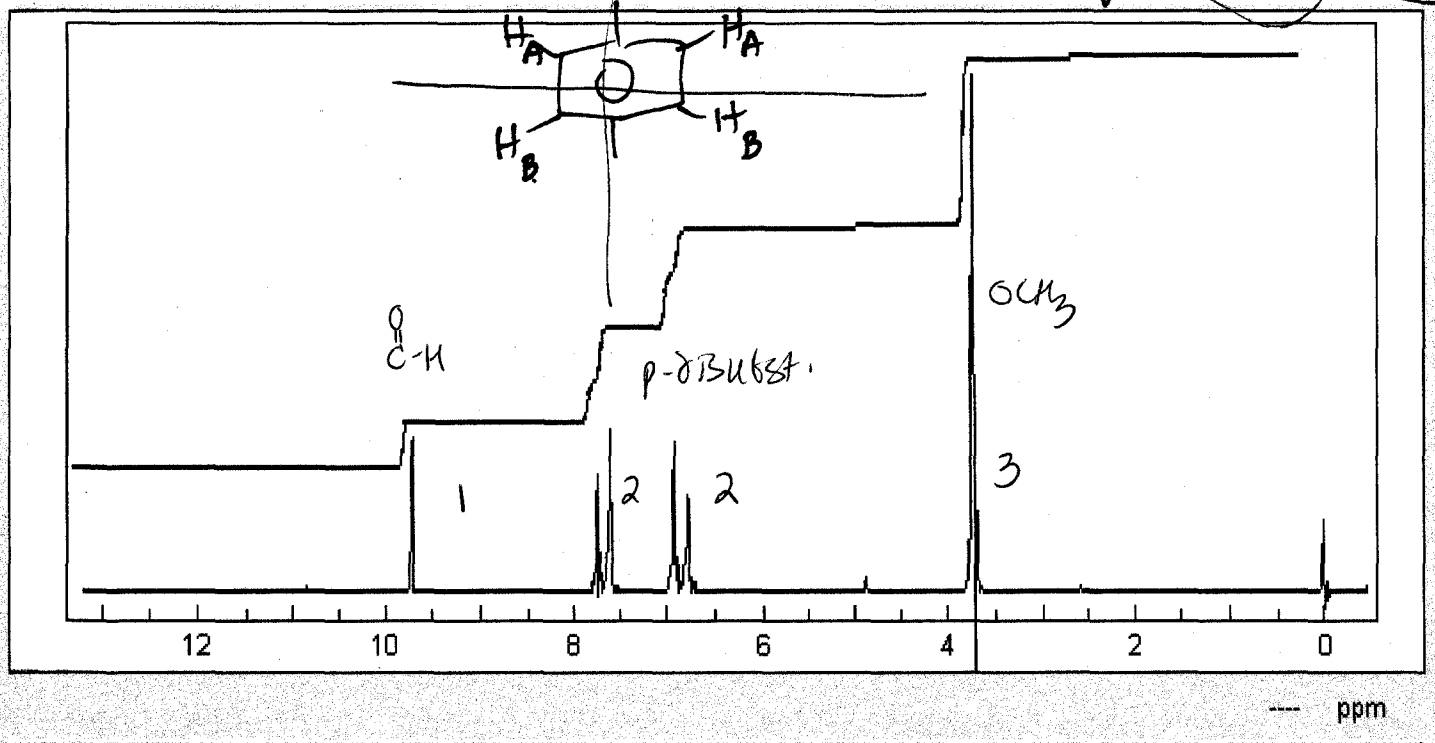
4 : 4 : 1 x 2

$C_8H_8O_2$

SODAR = 5

Disubst. benzene - possibilities:



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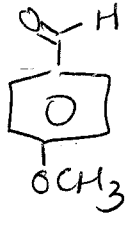
5.88 : 5.92 : 1.47

4 : 4 : 1

$C_4H_4O$ x2 $C_8H_8O_2$



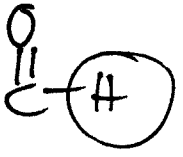

SODAR = 5

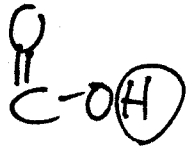
# Useful Numbers to Remember

~1 ppm $CH_3$'s ] $CH_2$, CH

~5 ppm alkenes ]

~7 ppm benzene/aromatics

~9 ppm aldehyde 

~12 ppm carboxylic acid 

attached to e⁻neg atom (O, N, X) → downfield

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

[ $-CH_3$ ~1 ppm  ~2.5 $-OCH_3$ ~4 ]