Answers

CHEM*2070 **Test #1** **Feb. 7, 2012**

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Instructions:
- only answers in boxes will be marked. Use back of each page for scrap paper.
- units are *required* for *answers* only.
- please do *not* use pencil or red pen.

$h = 6.62608 \times 10^{-34}$ Js

$R = 8.31451$ JK^{-1} mol^{-1}

$k_B = 1.38066 \times 10^{-23}$ JK^{-1}

$c = 2.9979 \times 10^{8}$ $ms^{-1} = 2.9979 \times 10^{10}$ $cm\ s^{-1}$

$m_e = 9.10939 \times 10^{-31}$ kg

$N_A = 6.02214 \times 10^{23}$ molecules

Q1	5 /5
Q2	9 /9
Q3	5 /5
Q4	8 /8
Q5	6 /6
Total	33/33
	/

$$\bar{D} = \frac{h^3}{32\pi^4 m^2 r^6 k\bar{c}} \qquad \frac{n_J}{n_0} = (2J+1)\exp\left[\frac{-BhJ(J+1)}{kT}\right]$$

$$J_{max} = \left(\frac{kT}{2hc\bar{B}}\right)^{1/2} - 1/2 \qquad \mu_{AB} = \frac{M_A M_B}{(M_A + M_B)1000N_A}$$

1. Definitions.

Define the following terms as they apply to "Structure and Spectroscopy":
Note that an example is not a definition but can be used to illustrate a definition.
(maximum 2 sentences each; any more and you lose marks)

a) Internal Rotation:

Rotation of one part of a molecule with respect to another part of that molecule

b) Intramolecular interaction:

- an interaction (H-bonding, etc.) between different parts of the same molecule

or

- an interaction which ~~takes~~ occurs within a molecule.

c) Symmetric top molecule:

- a molecule where 2 moments of inertia are the same
- a molecule having a symmetry axis of C_3 or higher.

d) Anisotropically polarizable molecule:

See 2011 Q1 part d) !

e) isotopologues:

Molecules which differ in their nuclear isotopes.

[5 Marks]

2. Short Answer:

a) In what region of the electromagnetic spectrum does a microwave oven emit light?

Microwave!

or - GHz (10^9-10^{11} s^{-1})

or - mm-cm (λ)

- cm^{-1} is 1-100

b) What are 3 potential uses of microwave (rotational) spectroscopy?

i) Molecular structure determination

ii) dipole moment determination

iii) determination of gas sample temperature

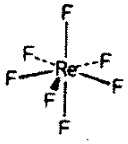
also - determination of bond force constant

- detection of gaseous extraterrestrial molecules

c) When is energy quantized?

when the motion of a particle is restricted

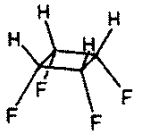
d) Indicate next to each molecule shown below if the molecule will give a microwave (MW), a rotational Raman (R), both (B), or neither (N).

i) 

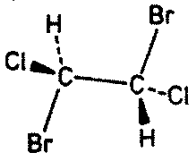
N

ii) 

B

iii) 

B

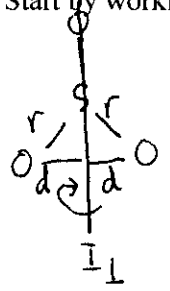
iv) 

R

[9 Marks]

3. Sulphur trioxide (SO_3) is a trigonal planar molecule with D_{3h} symmetry.
The rotational Raman spectrum of SO_3 is shown below. The spacing between the lines is 0.6974 cm^{-1}. Calculate the S – O bond length (in Å), r_{SO}. Hint: recall last year's midterm test.

Start by working out $I_\perp$

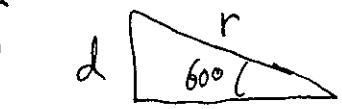


$I_\perp = 2 m_O d_O^2$

$d_O = r \sin 60°$

$d_O^2 = r_{SO}^2 \underbrace{\sin^2(60°)}_{3/4}$

$\therefore \boxed{I_\perp = \frac{3}{2} m_O r_{SO}^2}$



follow last year's exam exactly but with different numbers:

$$\Delta\nu = 2\bar{B} = \frac{2h}{8\pi^2 c I_\perp} = \frac{h}{6\pi^2 c m_O r_{SO}^2}$$

$m_O = \frac{15.9949}{1000\,(g/kg)\ 6.02214 \times 10^{23}\ molec/mol}\ (g/mol)$ ← see table on page 2 of exam

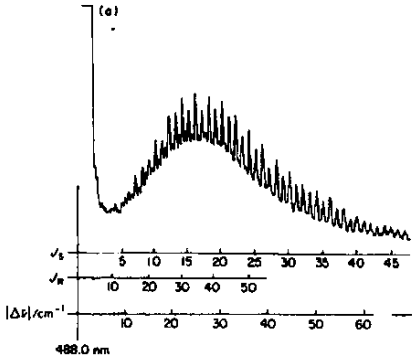
$$\therefore r = \sqrt{\frac{1000\,h\,N_A}{(6)\pi^2 c\,\Delta\bar{\nu}\,M_O}}$$

$$= \sqrt{\frac{(1000)(6.626 \times 10^{-34})(6.02214 \times 10^{23})}{(6)(9.8296)(2.9979 \times 10^{10})(0.6974)(15.9949)}}$$

$$= 1.422 \times 10^{-10}\ m$$

$$\boxed{r_{SO} = 1.422\ \text{Å}}$$

[5 marks]



4. Circle the preferred molecular conformation for each molecule and indicate in the box the dominant interaction (steric repulsion, hydrogen bonding or conjugation) which determines the preferred conformation.

a) 2-hydroxybenzaldehyde

H - bonding

b) 1,2-dichloroethane

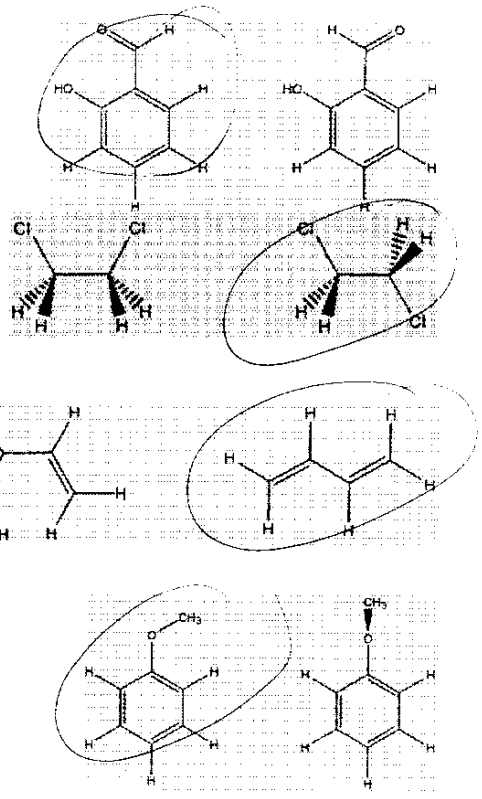
steric

c) Butadiene

steric

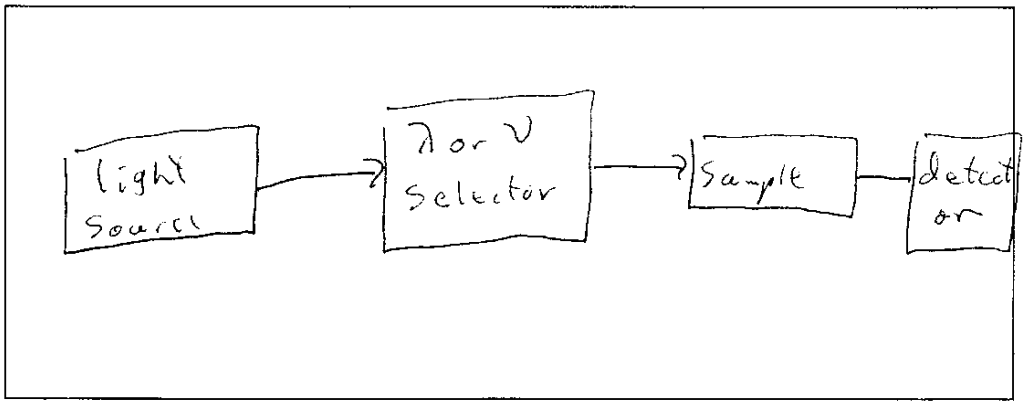
d) Anisole (done in class)

conjugation

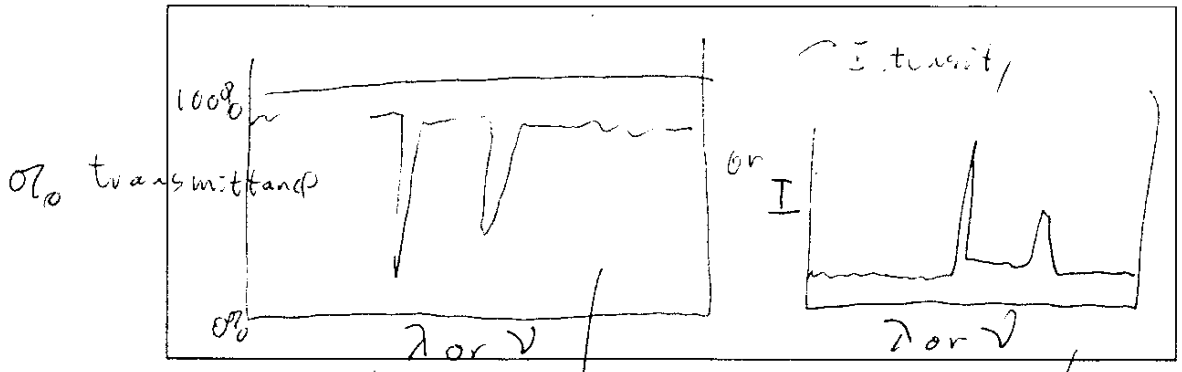


[8 Marks]

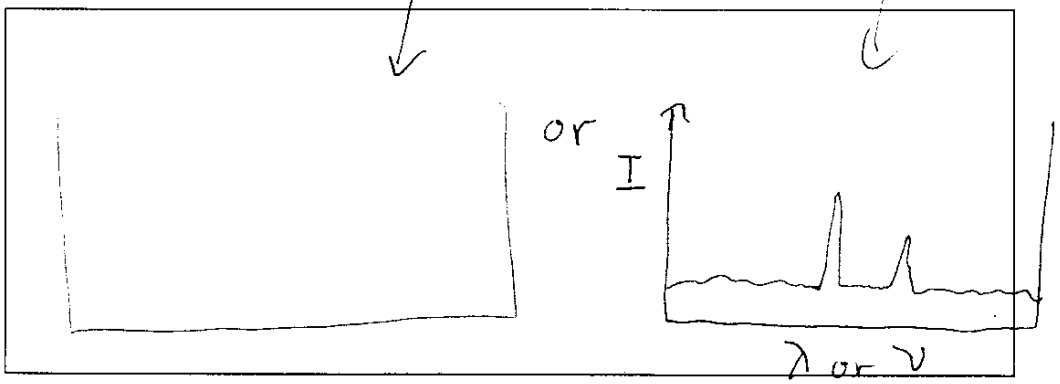
5. a) Sketch a basic ***absorption*** spectrometer (label all components).



b) Draw a typical *absorption/transmission* spectrum (label axes).



c) Draw a typical ***emission*** spectrum (label axes).



[6 Marks]