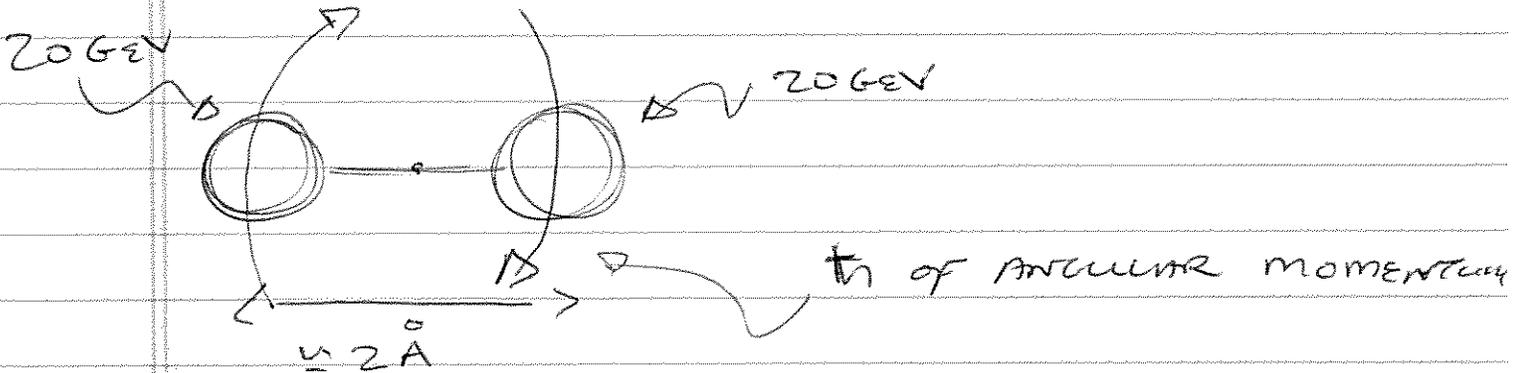


ANSWERS

(A1) CALCULATE THE FREQUENCY OF ROTATION OF A TYPICAL MOLECULE WITH ONE QUANTUM UNIT OF ANGULAR MOMENTUM (\hbar):



$$L = I\omega \implies \omega = \frac{L}{I} \quad \text{OR} \quad f = \frac{L}{2\pi I}$$

$$L = \hbar \quad (\text{ONE QUANTUM UNIT})$$

$$I = mR^2 + mR^2 = 2mR^2$$

$$m \approx 206 \text{ eV} \quad R = 1 \text{ \AA} \quad (\text{CENTER OF MASS IS HALFWAY BETWEEN})$$

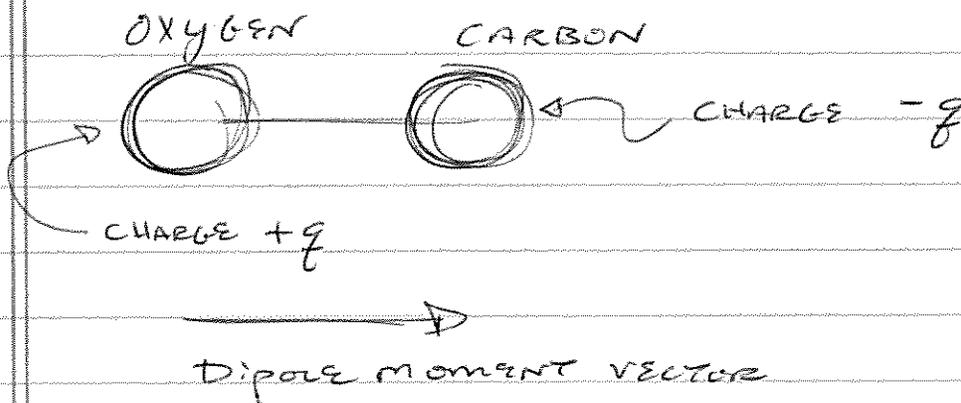
$$\implies f = \frac{\hbar}{2\pi \cdot 2mR^2} \cdot \frac{c^2}{c^2} = \frac{\hbar c}{4\pi m c^2 \cdot R} \cdot \frac{c}{R}$$

$$\left[\hbar c \approx 200 \text{ eV} \cdot \text{nm} \quad (\text{REMEMBER THIS!}) \right]$$

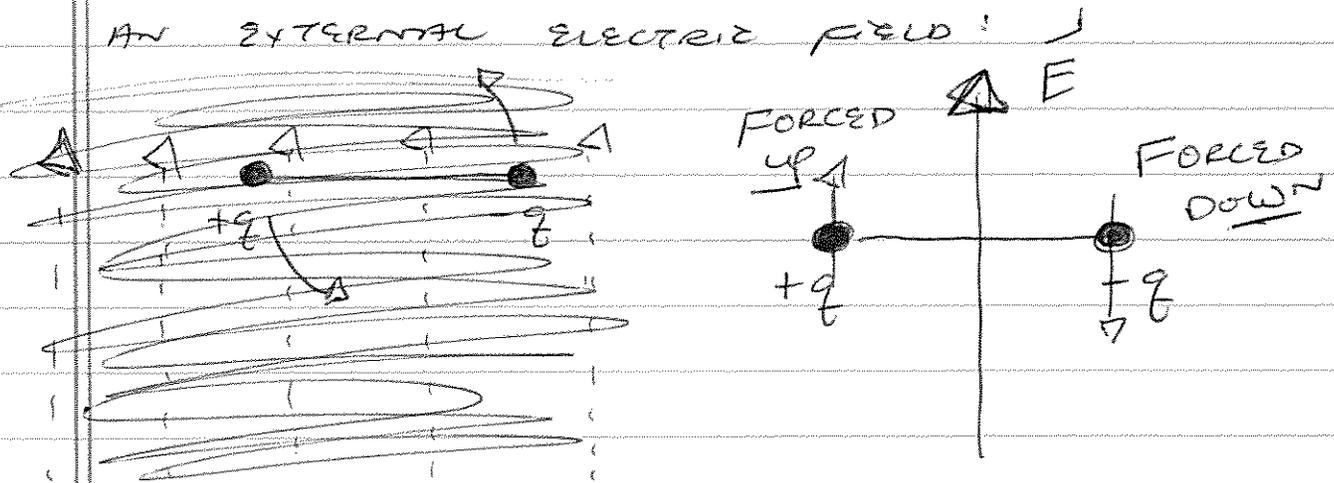
$$= \frac{200 \text{ eV} \cdot \text{nm}}{4\pi \cdot 206 \text{ eV} \cdot 1 \text{ nm}} \cdot \frac{10^9}{10^9} \cdot \frac{10^{10}}{10^{10}}$$

$$\approx 2.5 \cdot 10^{10} \text{ Hz} = 25 \text{ GHz}$$

NOW WHY A MOLECULE WOULD INTERACT WITH ELECTRO-MAGNETIC RADIATION AT ALL IS A SEPARATE QUESTION. MANY MOLECULES (INCLUDING CARBON MONOXIDE) HAVE SOME CHARGE SEPARATION IN THEIR NORMAL (EQUILIBRIUM) STATE. AMONG AS A RESULT SUCH MOLECULES POSSESS A NON-ZERO DIPOLE MOMENT. FOR DIATOMIC (TWO ATOM) MOLECULES THIS MOMENT POINTS ALONG THE BOND AXIS (WHERE ELSE, AFTER ALL, COULD IT POINT?):

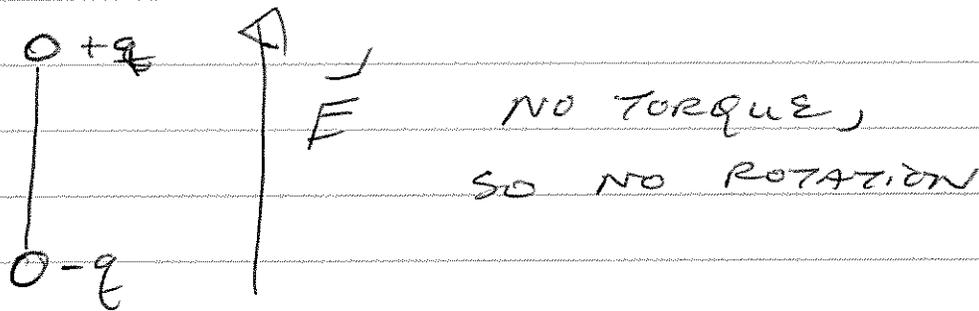


A DIPOLE WILL TRY TO ALIGN ITSELF WITH AN EXTERNAL ELECTRIC FIELD:



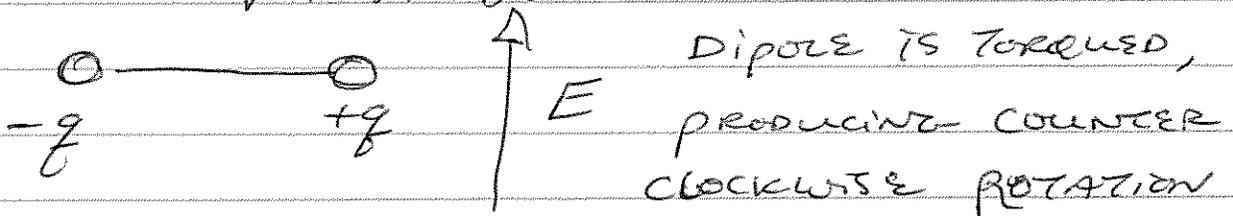
OR IN OTHER WORDS THE ELECTRIC FIELD WILL TORQUE THE MOLECULE, INDUCING ROTATION.

IF YOU SIMPLY APPLY A STATIC ELECTRIC FIELD, THE MOLECULE WILL ALIGN WITH THE FIELD AND STOP ROTATING:



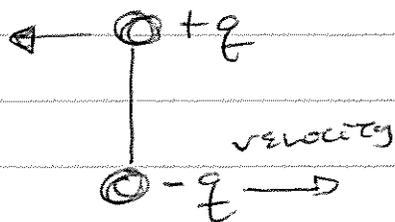
WITH AN OSCILLATING ELECTRIC FIELD (I.E. EM RADIATION) YOU CAN MAINTAIN ROTATIONAL MOTION. WE CAN SPLIT THE MOLECULE'S MOTION INTO FOUR STAGES:

FIRST STAGE:



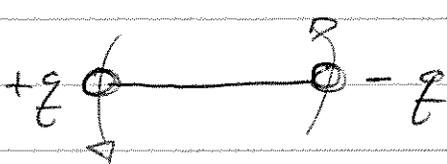
NEXT PAGE

velocity SECOND STAGE:



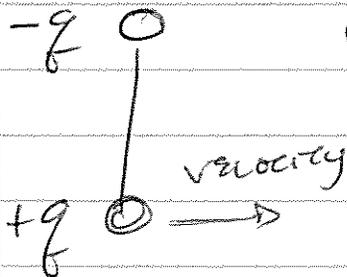
Dipole HAS SWUNG AROUND 90°
ELECTRIC FIELD IS TURNED
OFF. Dipole's ANGULAR
MOMENTUM KEEPS IT
ROTATING

THIRD STAGE:



Dipole HAS ROTATED 180°
ELECTRIC FIELD NOW
POINTING DOWN, WHICH
AGAIN TORQUES Dipole
COUNTER CLOCKWISE

velocity FOURTH STAGE:



~~stage~~

Dipole is @ 270° .
ELECTRIC FIELD IS TURNED
OFF AGAIN, ANGULAR
MOMENTUM SWINGS Dipole
BACK TO 360° , AND
WE START AGAIN @ THE
FIRST STAGE.

NOTE THAT IN THIS SCHEME THE MOLECULE WILL
ROTATE FASTER AND FASTER WITH EACH REVOLUTION
SO YOU WILL HAVE TO INCREASE THE RATE

AT WHICH YOU OSCILLATE THE ELECTRIC
FIELD IN ORDER TO STAY IN SYNC WITH
THE MOLECULE. IF YOU CAN DO THIS YOU
CAN ROTATE THE MOLECULE SO RAPIDLY THAT
IT WILL FLING ITSELF APART!

(A2) $B_{\ell}(\ell+1) \underline{u}$
 $\left(1 + \frac{\Delta r}{r_0}\right)^2$

$$B_{\ell}(\ell+1) \left[\frac{1}{\left(1+(0)\right)^2} + \frac{(-2)}{\left(1+(0)\right)^3} \frac{\Delta r}{r_0} \right]$$

(TAYLOR EXPANSION)

$$= B_{\ell}(\ell+1) \left[1 - 2 \frac{\Delta r}{r_0} \right]$$

(A3) $\left[\hbar \omega \left[a + a - + 1/2 \right] + B_{\ell}(\ell+1) \right] u_{n\ell}(r)$
 $= E_{n\ell} u_{n\ell}(r)$

THE $B_{\ell}(\ell+1)$ TERM IS ~~IS~~ CONSTANT W.R.T. ~~IS~~ Δr , SO ANY FUNCTION WILL BE AN EIGENFUNCTION OF THAT TERM.

THE EIGENFUNCTIONS OF $\hbar \omega \left[a + a - + 1/2 \right]$ ARE JUST THE HARMONIC OSCILLATOR EIG. FUNCS $\mathcal{Z}_n(\Delta r)$, SO LET:

$$u_{n\ell}(r) = \mathcal{Z}_n(r - r_0) = \mathcal{Z}_n(\Delta r)$$

THE EIGENVALUES $E_{n\ell}$ ARE THEN:

$$\hbar \omega \left(n + 1/2 \right) + B_{\ell}(\ell+1) = E_{n\ell}$$

$$\Delta E_l \equiv E_{0, l+1} - E_{0, l} =$$

$$\frac{\hbar\omega}{2} + B(l+1)(l+1+1)$$

$$- \frac{\hbar\omega}{2} - B(l)(l+1)$$

$$= B(l+1)(l+2-l)$$

$$= B(2l+2)$$

(A4)

$$B = \frac{\hbar^2}{2m^2 r_0^2} = \frac{(\hbar c)^2}{2mc^2 r_0^2}$$

$$\frac{2B}{\hbar} = 2B \cdot \frac{1}{\frac{\hbar c}{2\pi} \cdot \frac{2\pi}{c}} = \frac{c}{\pi} \cdot \frac{B}{\hbar c}$$

$$= 115816.04 \text{ MHz}$$

(A5)

YOU ALREADY CALCULATED SHIFT DUE
A LINEAR PERTURBATION IN LAST WEEK'S HW:

$$E_n^2 = \frac{-d^2}{2m\omega^2} \quad \text{WHERE} \quad H' = -dx$$

IN OUR CASE: $H' = -2B \frac{\Delta\Gamma}{\Gamma_0} l(l+1)$

SO AND $\Delta\Gamma \leftrightarrow x$ SO:

$$d = \frac{2B}{\Gamma_0} l(l+1)$$

$$E_{0l}^2 = \frac{-2B^2 (\hbar c)^2}{mc^2 (\hbar\omega)^2 \Gamma_0^2} l^2 (l+1)^2$$

$E_{0l}^2 = \frac{-2B^2 (\hbar c)^2}{mc^2 (\hbar\omega)^2 \Gamma_0^2} l^2 (l+1)^2$

$E_{0l}^2 = \frac{-2 (\hbar c)^5}{(mc^2)^3 (\hbar\omega)^2 \Gamma_0^2} c \cdot l^2 (l+1)^2$

$$E_{0l}^2 = -183.575 \text{ KHz} \cdot l(l+1)^2$$

$$h \cdot E_{0l}^2 = -0.183575 \text{ MHz} \cdot l^2 (l+1)^2$$

$$= -D l^2 (l+1)^2$$

D "STRETCHING CONSTANT"

2ND ORDER SHIFT IN TRANSITION FREQUENCY

$$\Delta E_l^2 = -D \left[(l+1)^2 (l+2)^2 - (l)^2 (l+1)^2 \right]$$

$$= -D (l+1)^2 \left[(l+2)^2 - l^2 \right]$$

$$= -D (l+1)^2 (l+2+l)(l+2-l)$$

$$= -4D (l+1)^3$$

2ND
ORDER
CORRECTION
TO
TRANSITION
SPACING

$$\Delta E_l^2 = \Delta E_{l+1}^2 - \Delta E_{l+0}^2$$
$$= -4D \left[(l+2)^3 - (l+1)^3 \right]$$

$$= l^3 + 4l^2 + 8l + 8 - l^3 - 2l^2 - 2l - 1$$

$$= 2l^2 + 6l + 7$$

$$= -4D (2l^2 + 6l + 7)$$