

Vibrational-rotation spectra

High resolution of gas phase heteronuclear diatomic shows that a single line may be divided into a number of closely spaced lines

vibrational and rotational changes

$$E_{v,J} = (v + \frac{1}{2})h\nu + hcB J(J+1) \quad \text{approximation}$$

vibrational transition	$v \rightarrow v+1$			
rotational transition	$J \rightarrow J-1, J, J+1$			
	$\Delta J = J_f - J_i$	-1	0	+1
	Branches	P	Q	R
	Energy	lower		higher

higher to lower  
 $1 \rightarrow 0$   
 $2 \rightarrow 1$

lower to higher  
 $0 \rightarrow 1$   
 $1 \rightarrow 2$

$\Delta E =$

$h\nu - 2BhcJ$

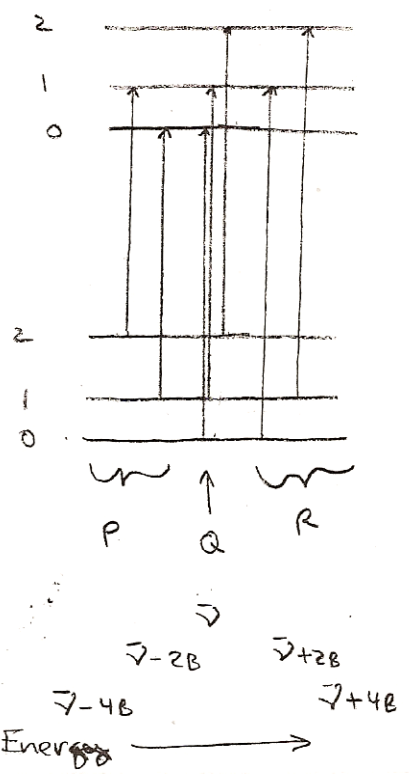
$h\nu$

$h\nu + 2Bhc(J+1)$

P starting level is also higher energy  
 $J = 1, 2, 3$

Q

R starting level is also lower energy  
 $J = 0, 1, 2$



can get rotational constant from vibrational infrared spectroscopy and thus bond length.

Q may be forbidden transition