Franck-Condon factor

We can use a T = 0 K approximation to calculate the Franck-Condon factor. In this approximation the molecules are in their electronic and vibrational ground state. Therefore, the FC transitions are from 0 -> 1', 0 -> 2', 0 -> 3', etc. The formula for this approximation is given by:

$$FC = \sum_{n=0'}^{\infty} \frac{S^n e^{-S}}{n!} \delta(\omega - \omega_{0-0'} - n\omega_{vib})$$

Calculate the "stick spectrum" by making a table showing the relative magnitude of the first 5 vibrational lines above 0-0'. You are given the follow information.

$$\omega_{0-0'} = 21{,}000\ cm^{-1}$$
$$\omega_{vib} = 1600\ cm^{-1}$$
$$S = 1.5$$

Franck-Condon factor

Method: All of the FC terms are multiplied by e^{-S}. Calculate that value, which is also the 0-0' FC factor and then multiply by $S^n/n!$. The corresponding transition energies shown in the table are given by

$$\omega = \omega_{0-0'} + n\omega_{vib}$$

n-> n'	FC	ω
0 -> 0'	0.223	21000
0 -> 1'	0.335	22600
0 -> 2'	0.251	24200
0 -> 3'	0.126	25800
0 -> 4'	0.047	27400

Franck-Condon factor

Next we can draw a “stick spectrum” based on the calculation in the table.