

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 $0 \rightarrow 0'$, $0 \rightarrow 1'$, $0 \rightarrow 2'$, 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 following information.

$$\begin{aligned}\omega_{0-0'} &= 41,000 \text{ cm}^{-1} \\ \omega_{vib} &= 900 \text{ cm}^{-1} \\ S &= 0.4\end{aligned}$$

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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'	FC	ω
0	0.670	41000
1	0.260	41900
2	0.053	42800
3	0.007	43700
4	0.001	44600

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