**Vibrational modes and IR spectral predictions using character tables**

The structure of SO2 may be deduced by its gas phase IR spectrum. Given that sulfur can expand its octet, theoretically either a bent (*C2v*) or linear (**) shape could be valid. For both structures, one would expect three vibrational modes: symmetrical stretch, asymmetrical stretch, and symmetrical bend. These three modes are shown below:



*C2v*

structure:

**

structure:

1. Bond length and angle changes take place during vibrations, but not every vibration absorbs IR energy as it vibrates. What must be happening during a particular vibrational mode if it is IR active?
2. Using the criteria from part (a), which of the three vibrational modes are expected to be IR active for each structure?

|  |  |
| --- | --- |
| Symmetry | Vibrational mode |
| Symmetrical stretch | Asymmetrical stretch | Symmmetrical bend |
| *C2v* |  |  |  |
|  |  |  |  |

1. Now using group theory reasoning (*C2v* and ** character tables are provided), determine which of the three vibrational modes are expected to be IR active for each structure.
2. The experimental IR spectrum of SO2 has three strong absorption bands at 1336, 1151, and 519 cm-1. In light of this experimental evidence and your analysis in parts (b) and (c), which point group is best supported? Also include reasoning regarding why the other point group is not likely.