Vibrational Modes and IR Spectra

The structure of SO2 may be deduced by its gas phase IR spectrum. Given that sulfur can expand its octet, theoretically either a bent 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. “Dance” each vibrational mode with some part of your body. Work with a partner to write out the two extremes of each vibration and decide the direction and relative magnitude of the dipole moment as the molecule vibrates. Once you have reached a consensus with another team, determine which of the above vibrational modes are expected to be IR active. Indicate Yes or No for each mode for each possible structure.

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

1. The experimental IR spectrum of SO2 has three strong absorption bands at 1336, 1151, and 519 cm-1. According to your reasoning above, is SO2 bent or linear?
2. Is SO2 a greenhouse gas?