Vibrational modes of molecules

Normal modes of vibration:

Diatomic molecules can perform only one single vibration motion. The number of possible vibrational modes of *multiatomic* molecules can be calculated in the following way: each single atom can move to 3N spatial coordinates for N number of atoms. Therefore a system of N points of mass has 3N degrees of freedom available.
In three of these movements, however, the atoms do not shift themselves relative to one another, but they all move in the same direction, thereby simultaneously changing the position of the center of mass.

Degree of freedom:

The number of vibrational degrees of freedom is showing by **Z=3N-6** for nonlinear molecules and **Z = 3N-5** for linear molecules. A linear three atomic molecule like CO_2 has 4, a nonlinear three atomic molecule like H_2O has 3, NH_3,NH_4 and N_2O_4 have 6,9 and 12 independent vibrational coordinates, respectively.

Types of vibrations:

All atoms of a molecule oscillate with the same frequency and in phase. There are *stretching*- (change of bond length) and *deformation*-vibrations (change of bond angle) existing. They can be symmetric and antisymmetric.

Examples:

Normal modes of vibration of CO_2 :

Vibration	Wave number cm^{-1}	Vibrational mode
V_1	1340	symmetric C=O stretching vibration
V_2	2349	antisymmetric C=O stretching vibration
V_{3a}	667	deformation vibration, two-fold degenerate
V_{3b}	667	

Normal mode of vibration of H_2O:

Vibration	Wave number cm^{-1}	Vibrational mode
V_1	3657	symmetric stretching vibration
V_2	1595	antisymmetric deformation vibration
V_3	3756	antisymmetric stretching vibration

Note : For a polyatomic molecul, some normal modes of vibration are spectroscopic active and some are not. The cross selection rule defines that the displacement of a normal mode must cause change in the dipole moment in order to be spectroscopically active in infrared.

Questions:

1) What is the cross selection rule for a polyatomic molecule to be active in IR spectroscopy?
2) How many vibrational modes CO_2 molecule has? Please sketch the symmetric, antisymmetric and deformation vibration modes of CO_2 molecule.

Literature:

- Helmut Günzler, Hans-Ulrich Gremlich, IR-Spectroscopy
- Shriver, Atkins, Inorganic Chemistry