CHEM 535	**Pavel Jungwirth**
Problem Set #6	April 27, 2006
	due May 3 in class

1) Predict, using group theory, the number of IR-allowed fundamental transitions in all possible triatomic molecules: linear (symmetric and non-symmetric) and bend (symmetric and non-symmetric).

2) Using vibrational constants for water (see below) calculate the frequencies of the following transitions: 000 → 100, 000 → 201, and 000 → 030.

$\nu_1 = 3825\ cm^{-1}$	$x_{11} = -44\ cm^{-1}$	$x_{12} = -20\ cm^{-1}$
$\nu_2 = 1654\ cm^{-1}$	$x_{22} = -20\ cm^{-1}$	$x_{13} = -155\ cm^{-1}$
$\nu_3 = 3936\ cm^{-1}$	$x_{33} = -46\ cm^{-1}$	$x_{23} = -20\ cm^{-1}$