Interaction of vibrational fundamental and combination states of ethylene in 3 μm region

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Formalism of symmetry groups has been developed and applied to expand the vibrational-rotational Hamiltonian and operator of dipole moment of ethylene into a power series of annihilation and creation operators as well as angular momentum operators. This approach allows to characterize every term of the series by its specific order in which the operators appear.

The first analysis of the 3 μm spectra reveals the strong coupling between ν_9, ν_{11}, $\nu_2+\nu_{12}$ and $2\cdot\nu_{10}+\nu_{12}$ yielding shifts of about 0.01 cm^{-1} for some low J and K lines of C_2H_4. We find that significant shifts are due to perturbations of ν_9 rotational-vibrational levels via 3^{rd} order b-type Coriolis interaction with the $\nu_3+\nu_8+\nu_{12}$ rotational levels.

A prominent borrowing of transition dipole moment is predicted for some otherwise dark rovibrational lines of the $\nu_3+\nu_8+\nu_{12}$ band. These satellite lines have been found and assigned in low temperature spectra of ethylene recorded by the F-center laser spectrometer in a jet and afterwards in room temperature spectra recorded earlier by the difference-frequency laser spectrometer [1] and recently by the FTIR spectrometer in the Giessen group. The fitting of interaction parameters with the mentioned perturbations leads to a standard deviation of $2\cdot 10^{-3}$ cm^{-1}, for low J lines of ethylene. The leading coupling parameters in the pentade ν_9, ν_{11}, $\nu_2+\nu_{12}$, $2\cdot\nu_{10}+\nu_{12}$ and $\nu_3+\nu_8+\nu_{12}$ are shown in the table

States	**Type**	**Value** (cm^{-1})
ν_{11} and $\nu_2+\nu_{12}$	cubic anharmonicity	45.459(2)
$\nu_2+\nu_{12}$ and $2\cdot\nu_{10}+\nu_{12}$	cubic anharmonicity	-10.721(2)
ν_9 and ν_{11}	1^{st} order Coriolis interaction	-0.130(3)
ν_9 and $\nu_3+\nu_8+\nu_{12}$	3^{st} order Coriolis interaction	-0.022(8)

The last parameter approximately describes, too, the perturbations between $\nu_9+\nu_{10}$ and $\nu_3+\nu_8+2\cdot\nu_{10}$, observed in the hot bands spectra.

[1] A.S.Pine *Tunable Laser Survey of Molecular Air Pollutants, Final Report* NSF/ASRA/DAR 78-24562, MIT, Lexington, Mass. (1980)