

## Comparison of Theoretical Intensity Calculations and Experimental Intensities Measurements for Non Linear Triatomic Molecules

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The knowledge of the infrared spectra of the atmospheric molecules is of the first importance for the atmospheric and metrological applications. Both measurements and calculations of lines intensities are necessary to complete spectroscopic databases.

Intensity calculations can be performed in different ways : one employs variational [1, 2] or DVR [3] methods using *ab initio* dipole moment functions, another one relies on effective spectroscopic models involving empirically determined *transition moment parameters* [4-6] specific for individual rovibrational bands. We report recent results based on a synthetic approach [7, 8] that allows a derivation of accurate values of transition moment parameters for ro-vibrational bands from molecular potential energy surface and dipole moment functions for non-linear triatomic molecule of the  $C_{2v}$  and  $C_s$  symmetry groups. Predictions of transition moment band parameters in case of isotopic substitutions including a symmetry breaking one:  $C_{2v} \rightarrow C_s$  will be discussed.

Comparisons between the theoretical intensity calculations and the experimental measurements for non-linear triatomic molecule of the  $C_{2v}$  and  $C_s$  symmetry groups as the water molecule  $H_2O$  and the deuterated sulphide hydrogen isotopologues  $D_2S$  and  $HDS$  will be presented. For the water molecule, these comparisons are possible as a lot of intensity data are available in the literature. Concerning the  $D_2^{32}S$  and  $HD^{32}S$  isotopologues, no intensity data were available, so we performed the first intensities measurement for the first and second triad bands [9]. The experimental intensities measurements were carried out by multispectrum fitting procedure [10] using the high resolution infrared spectra recorded with the Fourier transform spectrometer of Reims University. Comparisons between variational and algebraic methods of calculations are also discussed.

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