THEORETICAL STUDY OF THE ANOMALOUS BAND INTENSITY PROFILE OF THE $\nu_3 + \nu_5$ BAND OF SF_6

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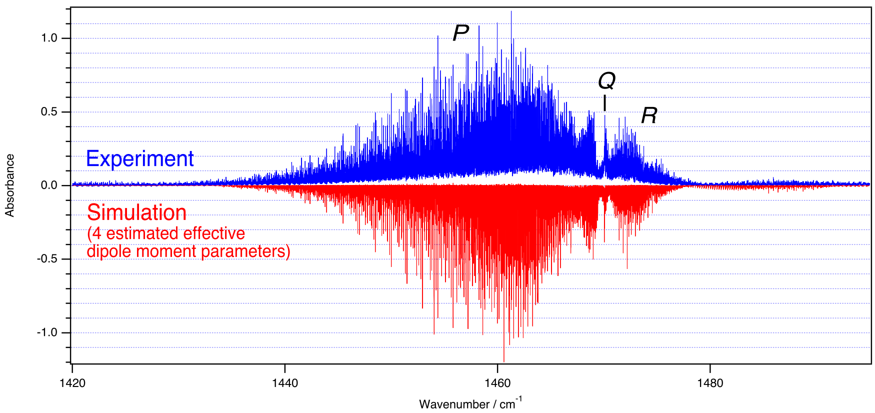
As part of an extensive study of the high-resolution infrared spectroscopy of the SF_6 molecule, Faye *et al.* have revealed the very unusual band intensity profile of the $\nu_3 + \nu_5$ combination band[1]. This one is very asymmetric and consists of a huge P branch along with weak Q and R branches (see Figure below).

In order to explain this structure, we undertook a theoretical study about the development of the effective dipole moment operator $\widetilde{\mu}$ for the $\nu_3 + \nu_5$ band considered as isolated, using the contact transformation approach. Starting from the Hamiltonian operator, we have diagonalized the first order (H_1) terms that contain, in particular, Coriolis contributions. From this, we could deduce the expression of $\widetilde{\mu}$ via the first contact transformation. The experimental parameter values coincide well with calculations made using these expressions. The small differences can be explained by higher order terms (second contact transformation).

This study also allows to estimate the zero order parameter of the untransformed dipole moment operator for the $\nu_4 + \nu_5$ and $\nu_5 + \nu_6$ combination bands.



Experimental *vs.* simulated spectrum of the $\nu_3 + \nu_5$ band of SF_6.

[1]M. Faye, L. Manceron, P. Roy, V. Boudon and M. Loëte, *J. Mol. Spectrosc.* **348**, 37–42 (2018).