

Hindered Rotation in the Infrared Spectra of HCl in Liquefied Rare Gases

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Infrared spectra of hydrogen halides in non polar solutions have been widely analyzed as a prototype of changes in the spectra of molecules in solution.

The more intriguing fact is that together with the P and R branches, which correspond to the envelopes of the low density gas spectra, it appears a central prominent resonance (Q branch) in the region where absorption is forbidden by the rotational selection rules for the isolated molecule.

The nature of the Q branch has been object of discussion along the last decades, and a large list of both theoretical and experimental works have been developed around this matter.

In a recent work [1] it has been proved that this Q branch is shifted from the vibrational fundamental frequency, being this shift correlated with that of the stretching mode of the $\text{HX}\cdots\text{solvent}$ Van der Waals complex.

A second effect discussed in that work is that the intensity of the Q branch is correlated with the loss of intensity of the region corresponding to transitions between the lower energy rotational states, and a simplified model was developed to reproduce the corresponding profiles.

In this model it is assumed that the solute molecule is able to rotate freely in the liquid, only when the sum of its translational and rotational energy is greater than the potential barrier corresponding to the anisotropic interaction between the solvent and the solute molecules.

The objective of this work is to show how this effect can also be seen in the far infrared spectra, comparing those of the HCl in Ar, Kr and Xe at different temperatures, and to analyze the comparative results between the pure rotational and vibration-rotation spectra.

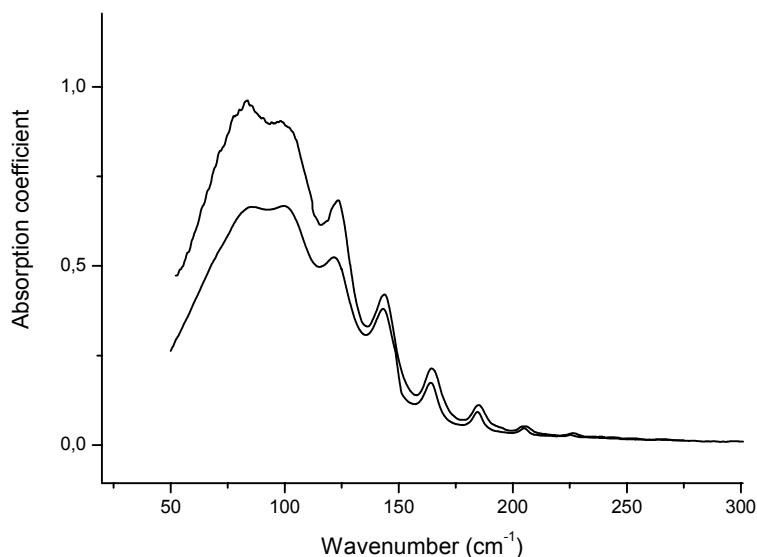


Fig. 1: Far infrared spectra of HCl in liquid Kr (top) and Xe (bottom) at $T = 165$ K [2].

[1] J. Pérez, A. Padilla, W.A. Herrebout, B.J. Van der Veken, A. Calvo Hernández and M.O. Bulanin. *J. Chem. Phys.* 122 (2005) 194507.

[2] W. Herrebout, B.J. Van der Veken, A. Medina, A Calvo Hernández and M.O. Bulanin. *Mol. Phys.* 96 (1999) 1115.