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ROTATIONAL ISOMERISM IN FLUORINATED COMPOUNDS: 1,3-DIFLUORO-2-CHLOROPROPANE

G. A. CROWDER

Department of Chemistry, West Texas State University, Canyon, Texas 79016 (USA)

SUMMARY

Infrared spectra were obtained for 1,3-difluoro-2-chloropropane in the solid, liquid and vapor states and in solutions with nonpolar solvents. Comparisons of the spectra show the probable presence of three conformations in the liquid, two in the solid, and only one in the vapor. Changes in relative intensities of several bands in nonpolar solvents show the less polar conformation to be the one present in the vapor state.

Rotational isomerism has been shown to exist in 1,3-difluoro-2-propanone [1] and 1,3-difluoro-2-propanol [2]. Both compounds were shown to exist as two conformations each. Those compounds are structurally similar to 1,3-difluoro-2-chloropropane, so the conformational behavior of this compound is of interest.

Infrared spectra of 1,3-difluoro-2-chloropropane in the liquid and vapor states are shown in Figs. 1 and 2. It can be seen that several liquid-state bands are absent in the vapor-state spectrum, showing the disappearance of one or more conformers upon vaporization. There are several pairs of bands present in the liquid-state spectrum that can be used to determine the relative polarities of the two conformations that give rise to the bands (e.g., 711, 722; 1305, 1317 cm^{-1}). The IR spectrum of the compound dissolved in the nonpolar solvent CS_2 (or CCl_4) shows the 722 cm^{-1} band, which is merely

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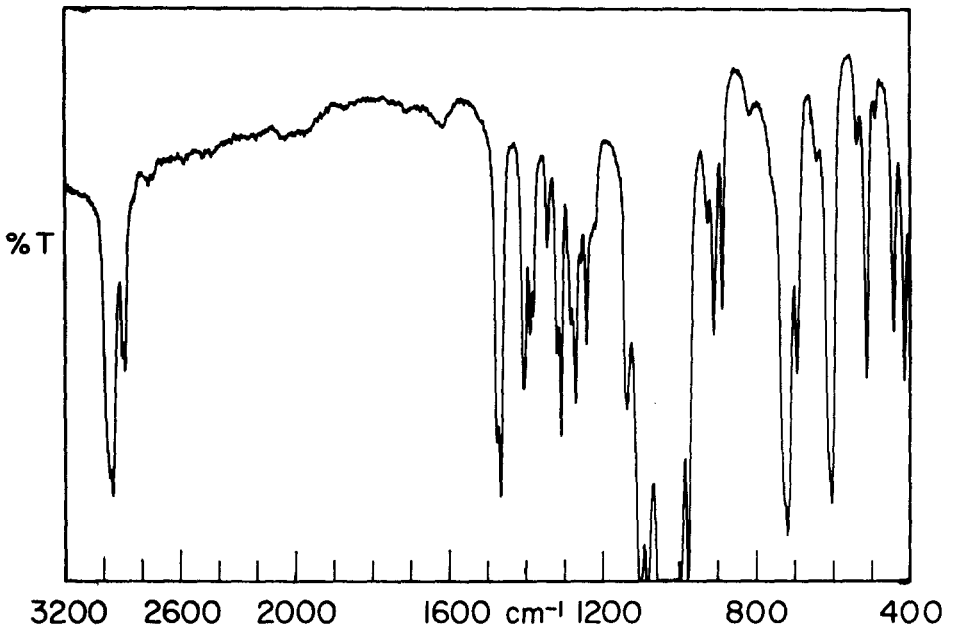

Fig. 1. Liquid-state infrared spectrum of $CH_2FCHClCH_2F$.

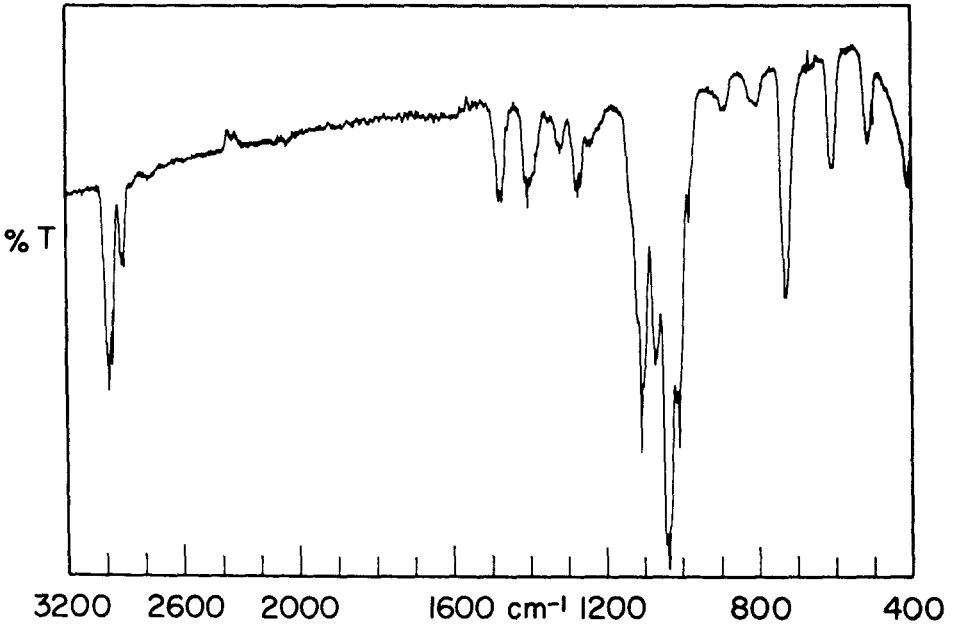

Fig. 2. Vapor-state infrared spectrum of $CH_2FCHClCH_2F$.

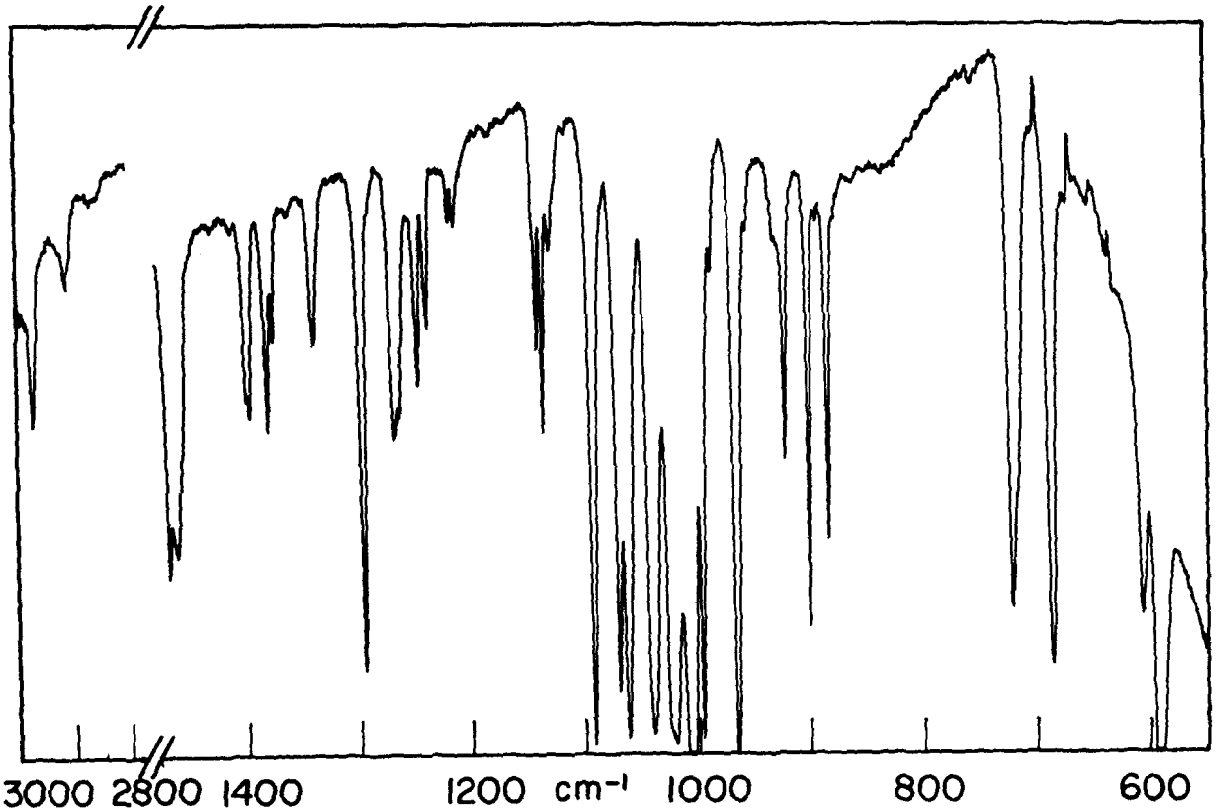

Fig. 3. Solid-state IR spectrum of $CH_2FCHClCH_2F$ at ca. 80K.

a shoulder on the more intense 711 cm^{-1} band in the liquid-state spectrum, is of equal intensity to the 711 cm^{-1} band. Likewise, the 1317 cm^{-1} band increases in intensity in the solution, which shows those two bands (722 and 1317 cm^{-1}) to be due to the less polar conformer. The intensities of several bands are obviously less in the spectrum of the CS_2 solution relative to that of the liquid, whereas the intensities of some bands change very little. The liquid-state band at 688 cm^{-1} is one whose intensity obviously decreases in nonpolar solvents, and it must be due to a more polar conformation.

The IR spectrum was also obtained for the compound in the solid state at ca. 80K. Several liquid-state bands are absent in the solid-state spectrum, including those at 722 and 1317 cm^{-1}, which shows the less polar conformer to be absent in the solid. The solid-state spectrum shows too many bands to be due to only one conformer, and it is therefore likely that two conformers are present. The solid probably was not crystalline.

The presence of only one conformer in the vapor state shows the less polar conformer to be more stable than the others by several kilocalories per mole. This was also the behavior of 1,3-difluoropropanone [1] and fluoropropanone [3], which showed the presence of only the less polar conformer in the vapor state. In contrast to this behavior, 1,2,3-trichloropropane and 1,2,3-tribromopropane both show the presence of three conformers in the vapor state [4], although one of the less polar conformers is considerably more abundant than the others.

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