THE COMMON CHLORINE NUCLEAR ELECTRIC QUADRUPOLE COUPLING TENSOR FOR ACYL CHLORIDES

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We have determined the complete ^{35}Cl and ^{37}Cl nuclear electric quadrupole coupling tensors for two conformers of valeroyl chloride, CH_3-$(CH_2)_3$-COCl, using pure rotational spectroscopy. These tensors have been diagonalized into the principal axes and compared with chlorine principal quadrupole coupling tensors for a number of simple acyl chlorides. In general the components of the chlorine principal quadrupole coupling tensor, and in particular χ_{zz}, are invariant to the organic group attached to the acyl chloride. It is evident, and not surprising, that the carbonyl of the acyl chloride functional group dominates the electric field gradient at the chlorine nucleus. We have found a common, acyl chloride functional group, ^{35}Cl χ_{zz} value of -59 $\pm$ 1 MHz. These findings will be discussed along with other work on tabulating common principal nuclear electric quadrupole coupling constants for relevant nuclei in simple organic functional groups[a].

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