C1

RECENT RESEARCH ON ISOTOPE EFFECTS IN HIGH RESOLUTION NMR SPECTROSCOPY

W. T. Raynes

Dept. of Chemistry, University of Sheffield, U.K.

Experimental studies of the effects of deuterium substitution on the magnetic shielding of carbon-13 nuclei and protons in the most of the compounds CH_nX_{4-n} (n=0-3, X=Cl,Br,I) give isotope shifts ranging from 0.25 ppb to 400 ppb. The shifts are explained in terms of vibrational averaging which gives slightly different mean molecular geometries for different isotopomers. For the methyl halides a more detailed interpretation is possible because of the availability of good harmonic and anharmonic force fields. The resolved carbon resonances from $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ are also quantitatively explained in term of different C-Cl bond lengths although it is necessary to go to second order to do so. For the resolved proton resonance the effects arising from the very slight changes in the C-H bond length and the interbond angle are found to be larger than the experimental error of ±0.03 ppb.

C2

RECENT APPLICATIONS OF MILLIMETER-WAVE AND SUBMILLIMETER-WAVE SPECTROSCOPY

Jean Demaison

Laboratoire de Spectroscopie Hertzienne, URA CNRS 249, Université de Lille I,
F59655 Villeneuve d'Ascq, France.

The different techniques in use in Lille for millimeter-wave and submillimeter-wave spectroscopy will be briefly described: harmonic generation, backward wave oscillators and far infrared laser sidebands. They will also be compared with techniques employed elsewhere. Applications of these techniques for measurement of rotational spectra will be presented. The determination of accurate centrifugal distortion constants will be discussed. The usefulness of millimeter-wave and submillimeter-wave spectroscopy to determine off-diagonal terms in the rotational Hamiltonian will be shown on a few typical examples.