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ISOTOPE EFFECTS OF $^{34/32}S$ AND $^{37/35}Cl$ ON THE NUCLEAR SHIELDING OF FLUORINE-19 AND THEIR CORRELATION WITH BOND LENGTHS

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The isotope effect of $^{34/32}S$ on the NMR frequency of ^{19}F has been measured for a series of sulfur fluorine compounds. The one-bond low-frequency (high-field) isotope shift $^{1}\Delta^{19}F(^{34/32}S)$ shows a strong inverse dependence on the S-F bond distance. For example, the axial F atoms of the longer S-F bond in SF_4 and its derivatives give much smaller values than the equatorial ones which form a shorter S-F bond. From this correlation S-F bond distances of similar sulfur fluorine compounds can be predicted. The two-bond isotope shifts $^{2}\Delta^{19}F(^{34/32}S)$ in compounds of type F_3CS- and S=C(F)X depend analogously on the C-S bond distance (the C-F bond length is almost constant). Together with the correlations between the isotope effects $^{1}\Delta^{77}Se(^{13/12}C)$ [1] and $^{1}\Delta^{31}P(^{15/14}N)$ [2], respectively, and the corresponding bond lengths, it appears that the dependence of isotope shifts on bond distances is a general phenomenon that can be applied to a series of closely related compounds.

The two-bond isotope effect $^{2}\Delta^{19}F(^{37/35}Cl)$ shows that the influence of two ^{37}Cl atoms on the ^{19}F shielding is additive and the number of Cl atoms in a group can be determined from the isotope pattern of the highly resolved spectrum.

1 W. Gombler, J. Am. Chem. Soc. 104, 6616 (1982).

2 W. Gombler, R. W. Kinas and W. J. Stec, Z. Naturforsch. Part B, in press.