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NMR spectra of sulphur–fluorine compounds: analysis and simulation by novel program systems

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^{19}F NMR spectroscopy allows the unequivocal identification of molecular structures for various series of sulphur–fluorine compounds, e.g. that derived from S_2F_2, SF_4 and SF_6. Novel program systems have been written to provide efficient handling of symmetry concepts of chemical and magnetic equivalence involving single spins and composite particles with spins $I=\frac{1}{2}$ and $I>\frac{1}{2}$ in isotropic and anisotropic solutions. The examples shown in Table 1 have been selected from current literature [1].

The research group at Düsseldorf has developed DAISY [1], a program system for automated analysis and simulation of NMR spectra running with main-frame computers and workstations. A special version exists for the Bruker X.32 system. The simulators DSYMPC and DCYMPC [1] are available for PC under DOS. The most advanced version, WIN-DAISY [1], derived in part from WIN-NMR (Bruker), working with WINDOWS on a PC 486, was used to simulate the examples listed under Nos. 1–14 in Table 1.

Fig. 1 shows the simulated ^{19}F NMR spectrum of compound 6, $SF_4{=}CD_2$. The program WIN-DAISY rapidly

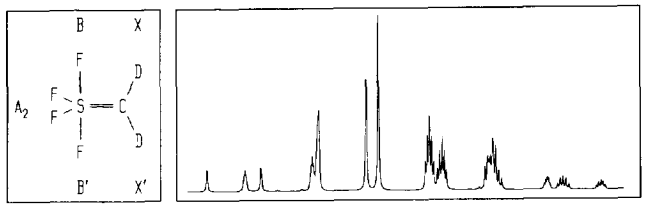

Fig. 1. 56.4 MHz ^{19}F NMR spectrum of $SF_4{=}CD_2$ simulated by WIN-DAISY. Limits of x axis: left: $\delta_F=64$ ppm; right; $\delta_F(B)=49$ ppm relative to $CFCl_3$ [2].

Table 1
List of compounds, spectra and spin systems

No.	Compound	Spectrum	Spin system	Spins	Groups
1	SF_3SCl	^{19}F, −100 °C	ABX	3	3
2	SF_3SF	^{19}F, −100 °C	AMRX	4	4
3	SF_4	^{19}F, −100 °C	A_2B_2	4	2
4	$SF_4{=}CH_2$	$^{19}F\{^1H\}$	A_2B_2	4	2
5	$SF_4{=}CH_2$	^{19}F, ^1H	$A_2[BX]_2$	6	5
6	$SF_4{=}CD_2$	^{19}F, ^2H	$A_2[B^1X]_2$	6	5
7	$SF_4{=}C(CH_3)CF_3$	^{19}F, ^1H	$A_2BCR_3X_3$	10	5
8	CF_3SF_4Cl	$^{19}F\{^{19}F\}$	AB_2C	4	3
9	SF_5Cl	^{19}F	AB_4	5	2
10	SF_5OPh	^{19}F	AB_4	5	2
11	S_2F_{10}	^{19}F	$[AB_4]_2$	10	4
12	$(SF_5)_2O$	^{19}F	$[AB_4]_2$	10	4
13	$(SF_5)_3N$	^{19}F	$[AB_4]_3$	15	6
14	$Hg(CF_3)_2$	^{19}F, ^{199}Hg, nema	$[A_3]_2$ and $[A_3]_2X$	6 and 7	2 and 3
15	SF_4	^{19}F, variable temp.	A_2B_2 dynamic	4	4

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calculates the $^{1/2}A_2[^{1/2}B^1X]_2$ spin system involving the deuterons with $I=1$. Equatorial fluorine atoms have a chemical shift of $\delta_F(A)=59$ ppm, while axial fluorines resonate at $\delta_F(B)=53.6$ ppm relative to $CFCl_3$.

Further PC programs designed in Düsseldorf [1] have been introduced for teaching NMR theory (MINILA), direct spectral analysis (SPINA-AT), LAOCOON-type iterations (LAOPC), cyclic simulations of NMR series (NMRFILM), double resonance studies (NMDR) and simulations of dynamic NMR spectra (DNMRSIM).

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