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AUTOMATED ANALYSIS AND SIMULATION OF ^{19}F-NMR-SPECTRA

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Modern preparative chemistry and studies of molecular structures in liquid or solution states require increasing amounts of explicite NMR data. A complete set of novel NMR programs based on group theoretical principles was designed, which will be helpful in practical chemistry for automated analysis and direct simulation ofHR-NMR-spectra, This new system was tested using organo fluorine compounds with data given in the open literature, from our own preparative studies or model systems from the research groups of A. Burg, D. Naumann and R.L. Soulen, which is gratefully acknoeledged. Basic principles and applications of our analytical tools are demonstrated with ^{19}F NMR spectra from the following fluorinated compounds:

1. Aromatic systems: 1,3,5-$C_6H_3F_3$, $C_{10}F_8$
2. Olefinic System: $CF_2{=}C(CF_3)_2$
3. Cycloaliphatic systems: cis/trans 1,2-$C_4F_6X_2$ (X = Br, Cl)
4. Cycloolefinic system: C_5F_8
5. Phosphorus derivatives: $N(PF_2)_3$, $(NPF_2)_3$

The method of automated analysis requires a digitized experimental band shape (spectrometer output) to find the resonance frequencies and coupling constants in isotropic or nematic phases using our programs SPECPREP, DAVSYM1, DAVSYM2, DAVCYM1 and DAVCYM2. Simulations are performed with DSYMPLOT and CYMPLOT. The programs will handle single spins or groups of spins with I greater or equal 1/2, so hetero nuclei ^{11}B, ^{95}Mo and others may be tackled as well. The programs are designed in Fortran IV to run on all IBM like computers. Copies are available on request from the authors.