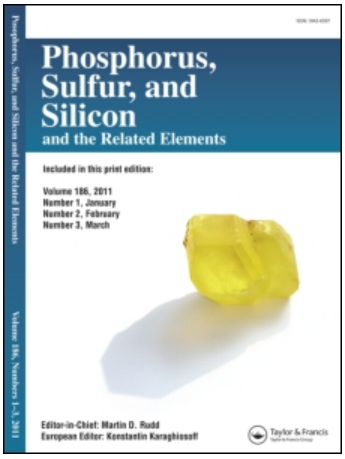

Phosphorus, Sulfur, and Silicon and the Related Elements

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Automated Analysis and Simulation of NMR Spectra: Applications to Organo Phosphorus Chemistry

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Automated Analysis and Simulation of NMR Spectra: Applications to Organo Phosphorus Chemistry

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Analysis of molecular structures in solution- and liquid-state is based on modern NMR methods. A novel set of computer programs was developed which allows for a more convenient automated analysis of NMR parameters and subsequent simulation of NMR spectra. Programs and techniques used are demonstrated for modelsystems like:

$RP(O)Cl_2$
$(RO)_2P(S)SH$ } R = C_2H_5, n-, i-C_3H_7, n-, i-, s-C_4H_9

$Ni(FPRR')_4$
$Mo(CO)_3(PF_3)_3$ } and related structures
$Mo(CO)_4(PF_3)_2$

Transfer of NMR spectra from spectrometer to PC computer is shown to obtain graphical output in high quality.
The methods demonstrated will be of general use for research and routine work done in university and industrial laboratories. The programs SPECPREP, DSYMPLOT, DCYMPLOT, DAVSYM1, DAVSYM2, DAVCYM1, DAVCYM2 and HERMES may be obtained on request from the authors.