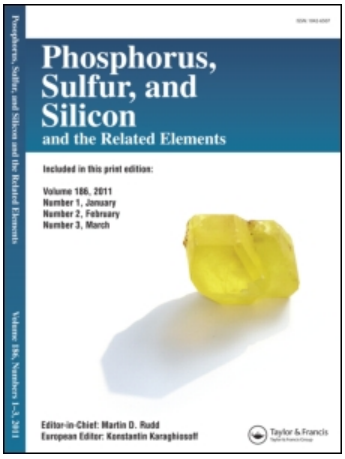


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# P-31 Solid State Nuclear Magnetic Resonance Investigations on Cyclophosphazenes

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# P-31 SOLID STATE NUCLEAR MAGNETIC RESONANCE INVESTIGATIONS ON CYCLOPHOSPHAZENES

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The present study deals with solid state NMR investigations on cyclophosphazenes with the following substituents: $-NH_2$, -OMe, -F, -Cl, -Br, at which the substituent atoms are elements of the 2nd period (N, O, and F) or elements of the 7th main group (F, Cl, and Br). The NMR spectra were obtained by a BRUKER MSL 300 spectrometer using a resonance frequency of 121.496 MHz. With each compound a static powder spectrum, a high speed MAS spectrum, and several side band spectra were recorded.

## RESULTS

The pattern of a P-31 solid state spectrum is mainly caused by the anisotropy of the P-31 chemical shift.
By means of the analysis of spinning side band intensities the principal values of the chemical shift tensor ($\delta_{11}$, $\delta_{22}$, $\delta_{33}$) could be obtained. From that it is possible to get the parameters Isotropic chemical shift, Span (Anisotropy), and Skew (Axiality)[1]. In table I the results of the solid state NMR measurements are shown.

TABLE I Solid state NMR parameter for some cyclophosphazenes

| Compound | Isotropic chem. shift [ppm] | $\delta_{11}$ | $\delta_{22}$ | $\delta_{33}$ | Span [ppm] | Skew |
|---|---|---|---|---|---|---|
| $N_3P_3(NH_2)_6$ | 18.8 / 12.7 | 61.3 / 82.4 | 35.8 / 7.8 | -40.8/ -52.0 | 102.1/134.4 | 0.5 / -0.1 |
| $N_3P_3(OMe)_6$ | 21.8 | 57.9 | 21.8 | -14.3 | 72.2 | 0 |
| $N_3P_3F_6$ | 3.8 | 83.0 | 0.1 | -72.0 | 155.0 | -0.1 |
| $N_3P_3Cl_6$ | 19.6 | 75.0 | 43.0 | -59.2 | 134.2 | 0.5 |
| $N_3P_3Br_6$ | -44.3 | 29.0 | 10.0 | -173.0 | 202.0 | 0.8 |

Additionally, quantum chemical calculations by the IGLO method to determine the principal values and the orientation of the shielding tensor were carried out. The orientation of the axes in the case of the $N_3P_3Cl_6$ molecule[2] shows that $\delta_{33}$ is perpendicular to the Cl-P-Cl plane and decisively influenced by the conditions (electron density and distribution) in this plane. Thus, the influence of substituents is reflected especially in $\delta_{33}$.

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