Intermolecular Interactions of Xe Atoms Confined in One-dimensional Nanochannels of Tris(*o*-phenylenedioxy)cyclotriphosphazene as Studied by High-pressure ^{129}Xe NMR

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The pressure dependence of the ^{129}Xe chemical shift tensor confined in the Tris(*o*-phenylenedioxy) cyclotriphosphazene (TPP) nanochannel was investigated by high-pressure ^{129}Xe NMR spectroscopy. The observed ^{129}Xe spectrum in the one-dimensional TPP nanochannel (0.45 nm in diameter) exhibits a powder pattern broadened by an axially symmetric chemical shift tensor. As the pressure increases from 0.02 to 7.0 MPa, a deshielding of 90 ppm is observed for the perpendicular component of the chemical shift tensor $\delta_\perp$, whereas a deshielding of about 30 ppm is observed for the parallel one, $\delta_\parallel$. This suggests that the components of the chemical shift tensor, $\delta_\parallel$ and $\delta_\perp$, are mainly dominated by the Xe-wall and Xe-Xe interaction, respectively. Furthermore, the effect of helium, which is present along with xenon gas, on the ^{129}Xe chemical shift is examined in detail. The average distance between the Xe atoms in the nanochannel is estimated to be 0.54 nm. This was found by using $\delta_\perp$ at the saturated pressure of xenon, and comparing the increment of the chemical shift value in $\delta_\perp$ to that of a β-phenol/Xe compound.

Key words: High-pressure ^{129}Xe NMR; TPP; One-dimensional Nanochannel; Pressure Dependence; ^{129}Xe Chemical Shift Tensor.