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New approaches to understanding molecular mobility in metal phosphate materials perspective as biosensors, fuel cells, catalysts and anticancer drug delivers: NMR relaxation, from theory to practice

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Statement of the Problem: There is little systematic understanding of the motions of phosphate groups in layered metal phosphate materials applied in chemistry, industry, and nanomedicine for drug delivery. These motions can play an important role in heterogeneous metal phosphate catalysis, proton conductivity in phosphate materials, and interaction between the phosphate network and intercalated compounds including drugs and their releasing. The purpose of this study is to show how to characterize quantitatively correlation times of motions in the metal phosphate network and to determine their activation energies.

Methodology & Theoretical Orientation: phosphorus spin-lattice (T^1) and spin-spin (T_2) NMR relaxation time measurements in static and spinning samples of modified metal phosphates and their interpretation from the theory to the practice of solid-state NMR.

Findings: The suggested ^{31}P T_1/T_2 approach with combination of ^1H T_ρ times provide: To detect molecular motions in the solid phosphate network and to recognize their types as the low-frequency proton transfer with the correlation times of 10−5 s and the high-frequency rotation in P−OH groups with the correlation times of 10−8 s at room temperature.

Conclusion & Significance: Phosphorus NMR relaxation is a powerful tool for studies molecular motions in solids which can be successfully used even in the presence of paramagnetic impurities. Its application has been demonstrated at probing of a low-energy phenylene rotor in a layered tin(IV) phosphonate/phosphate material as an example of a system attractive to develop molecular machines and devices.

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