

SOLID-STATE HIGH-RESOLUTION NMR $K_2PO_3F \cdot KF$

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In melts of potassium monofluorophosphate and potassium fluoride the new compound $K_2PO_3F \cdot KF$ is formed at 850 °C. According to x-ray powder diffraction data this compound and $K_2SO_4 \cdot KF$ [1] are isostructural. Only one mole fluoride per mole monofluorophosphate reacts. Solid-state high-resolution ^{19}F NMR spectroscopy shows that different types of fluorine atoms exist in the investigated samples.

In solid-state NMR spectra natural broadening due to strong direct dipolar F-F interactions masks the chemical shift and indirect spin-spin coupling. To overcome this obstacle we used the multipulse technique (four pulse cycle WHH 4 with $\tau = 4,1 \mu s$). The shape of the resulting high-resolution ^{19}F NMR spectra of polycrystalline samples is dominated by the F-P coupling tensor as well as the ^{19}F chemical shift tensor. On the basis of the tensor data it is possible to differentiate the covalent bonded fluorine atoms from the ionic bonded ones and to get new insights into the structure of the title compound.