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NMR Study of the Spin-Peierls transition in TiPO $_4^1$ RAIVO STERN, IVO HEINMAA, ENNO JOON, NICPB, Tallinn, JOSEPH LAW, REINHARD KREMER, Max Planck Institut für Festkförrperforschung, Stuttgart, ROBERT GLAUM, Institut für Anorganische Chemie, Universität Bonn — We investigated the magnetic and structural properties of the quasi-one dimensional $3d^1$ -quantum chain system TiPO $_4$ ($J\sim965$ K) by NMR measurements. TiPO $_4$ undergoes two magnetostructural phase transitions, one at 111 K and the other at 74 K. Below 74 K, NMR detects two different 31 P signals and the magnetic susceptibility vanishes, while DFT calculations evidence a bond alternation of the Ti...Ti distances within each chain. Thus, the 74 K phase transition is a spin-Peierls transition which evolves from an incommensurate phase existing between 111 K and 74 K.

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