

Spin-Peierls transition in TiPO_4

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We investigated the magnetic and structural properties of the quasi-one dimensional $3d^1$ -quantum chain system TiPO_4 ($J \sim 965$ K) by magnetic susceptibility, heat capacity, ESR, x-ray diffraction, NMR measurements, and by density functional calculations. 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 density functional 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.