Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Local structure of spin Peierls compound $TiPO_4$: $^{47/49}$Ti and ^{31}P NMR study[1] RAIVO STERN[2], IVO HEINMAA, ALEXANDER LEITME, ENNO JOON, ALEXANDER TSIRLIN, Natl Inst of Chem Phy Bio, REINHARD KREMER, MPI Stuttgart, ROBERT GLAUM, Universitt Bonn — TiPO4 structure is made of slightly corrugated TiO2 ribbon chains of edge-sharing TiO6 octahedra. The almost perfect 1D spin Ti3+ chains are well separated by PO4 tetrahedra. By magnetic susceptibility and MAS-NMR measurements [1] it was shown that TiPO4 has nonmagnetic singlet ground state with remarkably high Spin-Peierls (SP) transition temperature. The high-T magnetic susceptibility of TiPO4 follows well that of a S=1/2 Heisenberg chain with very strong nearest-neighbor AF spin-exchange coupling constant of J=965K. On cooling TiPO4 shows two successive phase transitions at 111K and 74K, with incommensurate (IC) SP phase between them. We studied local structure and dynamics in TiPO4 single crystal using 47/49Ti and 31P NMR in the temperature range 40K to 300K, and determined the principal values and orientation of the magnetic shift tensors for 31P and 47,49Ti nuclei. Since 47,49Ti (S=5/2 and S=7/2, respectively) have quadrupolar moments, we also found the principal axis values and orientations of the electric field gradient (efg) tensor in SP phase and at 295K. In SP phase the structure contains 2 magnetically inequivalent P sites and only one Ti site. From the T-dependence of the relaxation rate of 31P and 47Ti nuclei we determined activation energy Ea = 550 K for spin excitations in SP phase.

[1]J. Law et al., PRB 83, 180414(R) (2011)
[2]Support from ETAg by PUT210 and IUT23-3 is acknowledged.

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Date submitted: 06 Nov 2015 Electronic form version 1.4