

Abstract Submitted
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^{29}Si NMR study of polycrystalline $\text{NaTiSi}_2\text{O}_6$ ¹ RAIVO STERN, RIHO RSTA, IVO HEINMAA, ENNO JOON, NICPB, Tallinn, ESTONIA, HARLYN J. SILVERLEIN, CHRISTOPHER WIEBE, Dept. of Chemistry, University of Winnipeg, CANADA — $\text{NaTiSi}_2\text{O}_6$ (NTSO) structure consists of quasi 1-D zig-zag chains of edge-sharing slightly distorted TiO_6 octahedrons. The chains are separated by SiO_4 tetrahedrons. At high T the distance between magnetic spin-1/2 Ti^{3+} ions in the chain is equal. At $T_c = 210$ K the compound undergoes orbital-Peierls transition. As a result, below 210 K TiO_6 chain becomes dimerized having diamagnetic singlet ground state. Neutron spectroscopy provided singlet-triplet gap value 615(35) K [*], $\mu\text{SR } 2\Delta = 700(100)$ K. Our ^{29}Si magic angle spinning NMR spectra show in paramagnetic region one single resonance with paramagnetic shift $K = 713$ ppm at 300 K. The shift slightly increases with decreasing T and has maximum $K = 796$ ppm at $T = 213$ K. Below T_c the resonance transforms into two lines with different paramagnetic shifts. At $T = 56$ K the spectrum shows 2 sharp lines with diamagnetic chemical shifts -84 and -101 ppm corresponding to 2 different Si sites in the low-T unit cell. T-dependence of ^{29}Si spin-lattice relaxation T_1 in $70 \text{ K} < T < 140 \text{ K}$ follows activation type T-behavior with $E_a = 300(20)$ K, which we ascribe to the splitting between the 2 lowest *d*-orbital energy levels.

* H. J. Silverstein et al., PRB 90, 140402(R) (2014).

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