29Si NMR study of polycrystalline NaTiSi2O6

RAIVO STERN, RIHO RSTA, IVO HEINMAA, ENNO JOON, NICPB, Tallinn, ESTONIA, HAR-LYN J. SILVERLEIN, CHRISTOPHER WIEBE, Dept. of Chemistry, University of Winnipeg, CANADA — NaTiSi2O6 (NTSO) structure consists of quasi 1-D zig-zag chains of edge-sharing slightly distorted TiO6 octahedrons. The chains are separated by SiO4 tetrahedrons. At high T the distance between magnetic spin-1/2 Ti3+ ions in the chain is equal. At Tc =210 K the compound undergoes orbital-Peierls transition. As a result, below 210 K TiO6 chain becomes dimerized having diamagnetic singlet ground state. Neutron spectroscopy provided singlet-triplet gap value 615(35) K [1], $\mu$SR $2\Delta$ =700(100) K. Our 29Si 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 Tc 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 29Si spin-lattice relaxation $T_1$ in 70 K < T < 140 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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