Na$_2$Cu$_2$Si$_4$O$_{11}$·H$_2$O: A new S=1/2 chain material with microporous structure  

ANTONIO MOREIRA DOS SANTOS, PAULA BRANDAO, FILIPE ALMEIDA PAZ, VICTOR AMARAL, JOAO ROCHA, CICECO, Chem. Dept., U. Aveiro, Portugal, MARGARIDA GODINHO, CFMC, Fac. Ciências, U. Lisbon, Portugal, ALEXANDER VASILIEV, Moscow State University — We report the first S=1/2 chain microporous silicate, Na$_2$Cu$_2$Si$_4$O$_{11}$·H$_2$O. This compound was synthesized hydrothermally and its structure determined through single-crystal X-ray diffraction. It consists of pyroxene-type chains of distorted edge sharing CuO$_6$ octahedra separated by SiO$_4$ tetrahedra and running parallel to Na$^+$ filled channels. Susceptibility data was fitted using the S=1/2 alternating exchange parameters and $J_1/K_b$ and $J_2/K_b$ were determined to be 102 K and 16 K respectively. The spin gap $\Delta$ was extracted from the low temperature data and decreases with increasing magnetic field, also $2\Delta/K_bT_{sp}= 3.9$ close to 3.53, the expected value for a Spin-Peierls transition. These observations seem to indicate that this system is a two step Spin-Peierls system where a structural dimerization, already present at room temperature, is followed by a magnetic transition at lower temperature.

Antonio Moreira dos Santos  
CICECO, Chem. Dept., U. Aveiro, Portugal

Date submitted: 04 Dec 2004

Electronic form version 1.4