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Understanding Hydrogen Bonding and Low-Energy Magnetic Excitations in $\mathbf{VOHPO_4{\cdot}\frac{1}{2}H_2O}$ J. CAO, J.T. HARALDSEN, J.L. MUSFELDT, University of Tennessee, J.R. THOMPSON, T. BARNES, University of Tennessee and Oak Ridge National Laboratory, M.-H. WHANGBO, North Carolina State University, S. ZVYAGIN, National High Magnetic Field Laboratory, C.C. TORARDI, DuPont Company — We report the variable temperature vibrational properties of the S=1/2, quasi-one-dimensional quantum Heisenberg antiferromagnet $VOHPO_4{\cdot}\frac{1}{2}H_2O$. Vibrational splitting points toward a weak local symmetry breaking near 180 K, and the low-temperature redshift of V-O and H-O related modes demonstrates enhanced low-temperature hydrogen bonding. Due to spin-orbit interaction, the singlet to triplet gap also appears in the infrared response. We compare this value to those obtained via magnetic susceptibility, electron-spin resonance, and neutron scattering, and we point out the existence of a spectral feature that supports weak interaction between traditional"isolated V-V dimers." Both magnon dispersion calculations and the experimental data suggest α=J$'$/J is $\sim$ 7%.

Jinbo Cao
University of Tennessee

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