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Inelastic Neutron Scattering Predictions for V^{4+} Molecular Magnets J.T. HARALDSEN, University of Tennessee, T. BARNES, University of Tennessee and Oak Ridge National Laboratory — The two vanadium compounds $(CN_3H_6)_4Na_2[H_4V_6O_8(PO_4)_4((OCH_2)_3CCH_2OH)_2]\cdot 14H_2O$ and $Na_6[H_4V_6O_8(PO_4)_4((OCH_2)_3CCH_2OH)_2]\cdot 18H_2O$ are thought to be magnetically well described as trimers of S=1/2 V^{4+} ions, with a Heisenberg magnetic interaction between pairs. They are respectively isosceles (two interactions equal) and general (all interactions different) spin trimers. Inelastic neutron scattering can be used to test the assumed interaction pathways in these materials through comparisons of the measured and predicted INS structure factors. In this theoretical contribution we present results for these INS structure factors, which should be useful for the interpretation of INS experiments planned on these materials. With sufficient energy resolution one may also be able to observe interactions between the trimers, which have several possible superexchange pathways. We also discuss theoretical bulk magnetic properties, and compare them with experimental results in the literature.

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