Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Color properties, hydrogen bonding and magnetic interactions in $(TBA)_3[Ni(NCS)_5]$[1] T. V. BRINZARI, O. A. -I. SWADER, J. L. MUSFELDT, University of Tennessee, C. TIAN, M. -H. WHANGBO, North Carolina State University, J. A. SCHLUETER, Argonne National Laboratory — We investigated the optical and vibrational properties of $(TBA)_3[Ni(NCS)_5]$ a pentacoordinate Ni compound, and compared the results with the more traditional hexacoordinate analog $(TEA)_4[Ni(NCS)_6]$. Based upon electronic structure calculations, color properties of this high spin complex can be understood in terms of the crystal field splitting of the d-orbitals and their strong hybridization with the ligands. Temperature dependent vibrational studies show an additional splitting and softening of some of the modes at low temperature, which indicates enhanced hydrogen bonding between sulfur centers and organic ligands at low temperature as well as weak structural phase transitions.

[1]This work is supported by the National Science Foundation.

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Date submitted: 27 Nov 2007 Electronic form version 1.4