Abstract Submitted
for the NES07 Meeting of
The American Physical Society

Group Theoretical Techniques in Analyzing Vibronic Spectra from Doped Crystals. NICHOLAS APROBERTS-WARREN, JOHN COLLINS, Wheaton College — In this work we consider the use of vibronic spectra of rare earth and transition metal ions in ionic crystals to gain information on the phonon density of states. The impurity ion destroys the translational symmetry, leading to vibronic sidebands to emission lines that resemble the density of states. We focus on the application of selection rules for vibronic transitions to select crystals. Using group theoretical techniques, the symmetry of a crystal's unit cell and Brillouin Zone lead to "irreducible representations" of the space group of the crystal. Each of these representations corresponds to specific phonon modes of the perfect crystal. To determine which phonon modes can interact with the ion, the space group representations are reduced in terms of the site symmetry of the impurity, after which the selection rules can be applied. The specific case of Vn^{2+} in MgO is examined, and the results are compared with neutron scattering, Raman, and infrared data. Selection rules are also found for the cases of Cr^{3+} in strontium titanate and in yttrium aluminum garnet.

John Collins
Wheaton College

Date submitted: 13 Apr 2007 Electronic form version 1.4