

1014-Q1-1433

Charles S. Holmes* (holmescs@muohio.edu), Mathematics and Statistics Dept., Miami University, Oxford, OH 45056. *Molecular Vibrations in an elementary linear algebra course with early eigenvalues.*

My goal over the last several years has been to overhaul the elementary linear algebra course to make this and other applications available to my classes. By doing minimal polynomials and eigenvalues early there is a little extra time to study symmetry groups in 2 and 3 space. In the last two weeks of the semester students study one of several modules. This presentation focuses on the molecular vibration module. For a molecule with n atoms we describe a vibration as a motion in $3n$ space and represent this motion by its derivative vector. Then we study the action of the symmetry group of the time average position model of the molecule on these vibration vectors. This process yields a $3n$ dimensional representation of the symmetry group that gives clues as to the observability of different vibrations. Spectroscopic information can often sort out which of several possible models is most likely for the molecule. This module makes connections between linear algebra and the book on molecular vibrations by Wilson, Decius and Cross. The presentation benefits from many earlier conversations with my colleague, Dr. Joseph Cantrell, now a chemist with NASA. (Received September 28, 2005)