

## Computer Algebra Application in Chemical Spectroscopy. Applications in Point Group Analysis of Molecular Vibration and Comprehensive Solving of Deceptively Simple Second Order Nuclear Magnetic Resonance

Mihai Scarlete, Gavin Heverly-Coulson, Starr Dostie, and Karl Gagnon

Department of Chemistry, Bishops University, Sherbrooke, Canada

This contribution summarizes the advances in the utilization of computer algebra to the analysis of the activity of molecular vibration in Fourier-Transform Infrared Spectroscopy, and in the solving of complex Nuclear Magnetic Resonance spectra. The computation vehicle for the Point Group Analysis of molecular vibration is a Symbolic Computation Engine (SCE). In the first section, various computation modules are presented, designed for applications ranging from undergraduate teaching, to more elaborated versions integrated as important functionalities in advanced molecular modeling techniques used for research purposes. Fully integrated, digital character tables for most of point groups relevant for chemical species are built in SCE-compatible, comprehensive libraries. The advantages of this approach in teaching include manipulation of virtual molecules, step-by-step solutions for freshmen level, and fast, preformatted templates helping students to gain routine and eventually gain mastery on the subject. A special emphasis is put on the mathematical background of the calculations handled in SCE-code, covering the building of matrices associated to symmetry operators, computation of symmetry operators, coding of symmetry operations, point group analysis method, and matrix manipulations. In the second section, we introduce the utilization of computer-algebra in the reversible modeling-solving of deceptive AA'BB' NMR-spectra. The analysis of these spectra is hardly approachable by direct inspection or regular calculation. The continuous change of the spectrum to the limiting cases, and compatibility with the series of solutions bridging the deceptive cases to the known algorithms are discussed.