POSSIBLE APPLICATIONS OF MODERN HEURISTICS TO THE ASSIGNMENT OF DENSE MOLECULAR SPECTRA

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The assignment of dense rovibronic spectra has constituted for years, and continues to constitute, a great challenge to the molecular spectroscopist. This is particularly true when the selection rules of the molecule are not very stringent, and in the presence of large-amplitude vibrational modes. The availability of powerful desktop computers has lead to the development of interactive assignment methods, like the use of spreadsheets and the Ritz program[a], and, more recently, to the first attempts to completely automate the interpretation of these spectra. Independently, during the last four decades there has been a growing interest in algorithms which rely on analogies to natural processes. These include, notably, simulated annealing, neural networks, genetic algorithms and ant algorithms. Most of these algorithms can solve complex maximization/minimization problems, notably χ^2 minimization. A first application of genetic algorithms to molecular spectroscopy was presented by W. L. Meerts[b] at this conference two years ago. In this contribution we discuss the possibility of exploiting one of the origins of the spectral complexity, namely the presence of non-stringent selection rules, for assigning a spectrum by minimizing the number of levels compatible with a given set of spectral lines (combinatorial minimization). Some preliminary results on artificial sets of more than 2 000 lines will be presented. The effects of experimental accuracy, and the possibility of searching for constrained minima, will be discussed.

[a] G. Moruzzi, Li-Hong Xu, R. M. Lees, B. P. Winnewisser and M. Winnewisser, J. Mol. Spectrosc., 167, 156–175 (1994).

[b] W. L. Meerts, J. A. Hageman, R. Wehrens, L. M. C. Buydens and R. de Gelder, 55th Ohio State University International Symposium on Molecular Spectroscopy, June 12-16, 2000, MI03.