APPLICATION OF THE GENETIC ALGORITHM IN THE ANALYIS OF COMPLEX MOLECULAR SPECTRA

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It has been shown[a] that the Genetic Algorithm can be used in the assignment of high density spectra. Since the method does not require an initial assignment of quantum numbers to the individual transitions it can be of great help in the analysis of complex spectra with many (partly) overlapping lines. The major requirement for the success of the technique is that the theoretical model is capable to predict both the positions and intensities of the spectrum.

High resolution rotational resolved UV-laser spectra form in general a perfect class of spectra to be analyzed by the Genetic Algorithm using an asymmetric rotor Hamiltonian.

One of the major drawbacks for application was the relatively large amount of computing time needed to perform a convergence calculation using the Genetic Algorithm. We have greatly improved the various algorithms to obtain the evaluation function[a] which is used as a criterium for the quality of the fit. Together with a few other improvements on the computing process this has resulted in a reduction of the computing time by a factor of 10. It is now within the scope of modern PC's, even with a single processor, to perform a full Genetic Algorithm convergence on a complicated spectrum over lunchtime. This can be done without any prior assignments of transitions nor knowledge of the parameters.

We will show results on previously investigated spectra of ^{18}O substituted phenol[b] and results on the Ne-benzonitrile cluster not previously assigned in the conventional way.

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[a] Direct Determination of Molecular Constants from Rovibronic Spectra with Genetic Algorithms. J.A. Hageman, R. Wehrens, R. de Gelder, W.L. Meerts and L.M.C. Buydens. J. Chem. Phys. 113 (2000) 7955-7962.

[b] The structure of phenol in the S_1-state determined by high resolution UV-spectroscopy. Ch. Ratzer, J. Küpper, D. Spangenberg and M. Schmitt. Chem. Phys. 283 (2002) 153