METHANOL AND THE LONG WAY TOWARDS AUTOMATED SPECTRAL INTERPRETATION

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High resolution Fourier transform (FT) molecular spectroscopy has always dealt with extermely large numbers of spectral lines. Hundreds of thousands of absorption lines are observed even in the FIR-IR (from about 20 to about 1000 cm^{-1}) FT spectra of small five-atom (e.g. H_2NCN) or six-atom (e.g. CH_3OH and all its isotopomers) molecules. The task of assigning such spectra has thus lead the researchers to develop "computer-aided" assignment techniques from the very beginning. In practice, all of these techniques rely on the fact that sequences of energy levels sharing all quantum numbers but J can be expanded into rapidly converging Taylor series in $J(J+1)$ truncated at low orders. This property is reflected onto the structure of line sequences in P and R branches. Historically, the first form of computer-aided line assignment was the use of commercial spreadsheets in order to follow P and R branches. This was followed by the development of programs expressly written for spectral assignments, notably the programs using the Loomis-Wood method[a]. Due to both its theoretical and practical interest much work of many research groups has been devoted to the assignment of the spectrum of methanol and its isotopomers. Two families of programs for the assignment of the methanol spectrum have been developed in Pisa. The first program family was based an the Taylor expansion of the energy levels, rather than the development of the lines[b], while the second is based on the Rydberg-Ritz combination principle and has recently been extended to other molecules, notably cyanamide[c]. However, all of these programs are still far from true automated spectral interpretation: all of them are highly interactive and rely on some starting assignments done by other methods. Some possibilities for further approaching this goal will be discussed.

[a] B. P. Winnewisser, J. Reinstädtler, K. M. T. Yamada, and J. Behrend, *J. Mol. Spectrosc.* **136**, 12–16 (1989).

[b] G. Moruzzi and F. Strumia, *Infrared Phys.* **24**, 257–260 (1983).

[c] G. Moruzzi, W. Jabs, B. P. Winnewisser, and M. Winnewisser, Analysis of the FIR Cyanamide Spectrum by the "Multi-Molecule" Ritz Program, paper presented at The 52nd Ohio State University International Symposium on Molecular Spectroscopy, Columbus, 1997.