A "MULTI-MOLECULE" RITZ PROGRAM

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The "Ritz" program, already presented in two previous Columbus Symposia [a] [b], has been extended to enable the treatment of molecules other than methanol and its isotopomers. The new program first reads an ASCII file with information specific to the molecule (quantum numbers, transition rules, approximate wavenumbers for the vibrational modes ...), then loads the databases for the molecule and enters an interactive mode. As the older "Ritz" program, the new "multi-molecule" Ritz program evaluates the energy levels involved in the assigned lines by the Rydberg-Ritz combination principle, then extrapolates the energies of new levels by parabolic extrapolation, or searches for them by "expert system" techniques. The program has already been tested with an investigation of the small-amplitude vibrational ground state of hydrazine. Full investigations of the IR-FIR hydrazine spectrum (in collaboration with Li-Hong Xu) and cyanamide and mehtyl-amine spectra (in collaboration with the Physikalisch-Chemisches Institut of the University of Giessen) are planned.

[a] G. Moruzzi and L. H. Xu, Ohio State University 49th International Symposium on Molecular Spectroscopy, TD04, p.122 (1994).
[b] G. Moruzzi and L. H. Xu, Ohio State University 50th International Symposium on Molecular Spectroscopy, FA02, p.325 (1995).