THE MULTIMOLECULE RITZ PROGRAM: RECENT IMPROVEMENTS

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The last two molecules investigated by the Ritz program, oxetane[a] and acetaldehyde, have lead to the introduction of new relevant options into the Ritz package. The difficulties encountered in the assignment of the Fourier-Transform FIR spectra of both molecules are due to the occurrence of important overlappings of weak lines, corresponding to low K values. The first new option is the possibility of fitting symultaneously the whole set of assigned lines to a set of Watson Hamiltonians in A reduction, with the further option of selecting any of the three representations I^r, II^r and III^r. The resulting feed-back has been vital for the assignment of the low K_c sequences ($0 \leq K_c \leq 2$) of oxetane belonging to the $v_{\mathrm{rp}} = 3, 4$ and 5 ring-puckering states. The development of a Hamiltonian reproducing the lowest fundamental band of acetaldehyde, ν_{10}, within the experimeltal errors is the goal of the investigation of this molecule, thus, an analogous approach for acetaldehyde is not possible at the moment. Rather, we have introduced a new graphical option which displays the deviation of the investigated level sequence from its best fit by a Taylor series in $J(J+1)$, truncated at the first or second power, on the monitor. By clicking on any of the fitted levels, it is possible to display the list of the lines connecting it to ground-state levels, to display the spectral region around each of these lines, and to search for new possible level values connected to the appropriate ground-state levels by transitions whose frequencies are found in the spectrum. The new deviations from the best fitting power series are immediately shown on the monitor. This has lead to the completion of the assignment of the A-symmetry species, filling the $|K| \leq 3$ gap present in a previous report[b], while the completion of the assignment of the E-symmetry species is in progress.

[a] G. Moruzzi, M. Kunzmann, B. P. Winnewisser and M. Winnewisser, Ritz Assignment and Watson Fits of the High-Resolution Ring-Puckering Spectrum of Oxetane, *J. Mol. Spectrosc.*, in press

[b] G. Moruzzi, I. Kleiner, N. Moazzen-Ahmadi, A. R. W. McKellar and J. T. Hougen, 54th Ohio State University International Symposium on Molecular Spectroscopy, Columbus, June 14–18, 1999, TF10