A NEW COMPUTER PROGRAM FOR THE ANALYSIS AND FITTING OF SINGLET- TRIPLET SPECTRA OF ORTHORHOMBIC ASYMMETRIC TOP MOLECULES IN THE PROLATE OR OBLATE LIMITS

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The original version of our singlet-triplet rotational least-squares/band contour analysis program [a] has been modified to run under Microsoft Windows using the C++ programming language. The new version takes full advantage of the graphical capabilities of the Microsoft Foundation Class. Specifically, windows can be created that edit the input file, summarize the results of the least-squares fit, display the calculated and observed spectra, display whole or partial sections of the calculated spectrum as a stick or Gaussian deconvoluted spectrum. A listing of the rotational quantum numbers in the case (a) and case (b) limits for each of the displayed lines is provided. A branch annotating routine provides a quick visual guide to the assignment of the spectrum. A new eigenvalue sorting method has been added as an option that complements the existing method based on the eigenvector coefficients. The new sorting method has eliminated some difficulties that may arise using the existing "Least Ambiguous Method". The program has been extended to handle near- oblate asymmetric tops using a type III^r representation. The talk will also focus on some of the problems that can arise when spin-spin and spin-rotation constants are refined within an inappropriate representation.

[a] R.H. Judge, E.D. Womeldorf, R.A. Morris, D.E. Shimp, D.J. Clouthier, D.L. Joo, D.C. Moule, Comp. Phys. Commun., 93, 241 (1996).