ASYROTWIN: A WINDOWS PROGRAM FOR THE ANALYSIS OF HIGH RESOLUTION SINGLET-SINGLET BAND SPECTRA OF ASYMMETRIC TOPS

RICHARD H. JUDGE, *Department of Chemistry, University of Wisconsin-Parkside, Kenosha, WI 53141-2000*; DENNIS J. CLOUTHIER, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

We have written a greatly enhanced Windows version of the venerable Asyrot program originally designed by F. W. Birss[a] as a general purpose least-squares fitting program applicable to the analysis of the rotational structure of vibrational and vibronic bands of asymmetric rotor molecules. The new version extends the computational limits to J = 999 and K_a = 450 and includes the octic, M_K, and N_K centrifugal distortion constants. The number of transitions calculated and fitted is limited only by available computer memory. Two new features have been added to the program so that the parameters of a single state can be refined by forming combination differences and then fitting them, along with any available microwave lines, to the appropriate Hamiltonian. A new Windows interface, with extensive help files, has been integrated with the Fortran code to greatly facilitate the editing of the input data. A limited Windows based band contour plotting and comparison feature has been added. Two utility features are also available. The first allows for the easy transfer of observed line frequencies to the corresponding transition quantum labels listed in the input file. The second allows for the summation of several calculated spectra, of different bands or isotopomers, into an overall contour which can be compared to an observed spectrum. The presentation will focus on a demonstration of these features. The program has been published[b] and the code is available from the Computer Physics Communications Program Library.[c]

[a] F. W. Birss and D. A. Ramsay, *Comput. Phys. Commun.* **38**, 83 (1984).
[b] R. H. Judge and D. J. Clouthier, *Comput. Phys. Commun.* in press (2001).
[c] http:www.cpc.cs.qub.ac.uk/cpc/