PRACTICAL APPLICATION OF ASYMMETRIC TOP-ASYMMETRIC FRAME INTERNAL ROTATION THEORY TO EXPERIMENTAL RESULTS ON ETHYL AND PROPARGYL ALCOHOL

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The torsion-rotation spectrum of ground states ethyl and propargyl alcohol have been successfully analyzed with an asymmetric top-asymmetric frame Hamiltonian to J=60 and J=80, respectively. The basic form of the internal axis system (IAS), reduced axis system (RAS), and principal axis system (PAS) Hamiltonians will be presented. In each case the axis system chosen dictates which portion of torsional Hamiltonian must be solved with the overall rotation. Experimentally all of these Hamiltonians are complicated and present a number of often hard to determine and highly correlated terms. Fortunately, crude structural calculations can often provide important insight into the form of the torsional problem, the size of the interactions and a convenient axis system. Ethyl and propargyl alcohol provide two examples of very different kinds of torsional motion. The experimental problems associated with application of torsion-rotation Hamiltonians in different axis systems to ethyl and propargyl alcohol will be presented.