ASSIGNMENT AND ANALYSIS OF LOW-BARRIER ASYMMETRIC TOPS WITH SPFIT/SPCAT

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The interstellar medium contains a cornucopia of organic molecules. Unfortunately, a number of these molecules have highly complex spectra that require great efforts to achieve the comprehensive spectral understanding that might allay the confusion presented by unidentifiable features expected from next-generation submillimeter telescopes. Pickett's program suite SPFIT/SPCAT[a] was developed to nurture the need for a cohesive and comprehensive database and, as such, has become the cornerstone of the two most utilized astrophysical molecular databases (JPL[b] and CDMS[c]). Over the last several years this highly versatile fitting program has undergone significant modification (Pickett developed a front-end program known as IAMCALC) in order to accommodate the generic hindered rotor. Two years ago we laid out the plan for comprehensive assignments of acetaldehyde, which had been systematically studied up to 0.6 THz with the Reduced axis system internal rotation code (Belgi)[d], and now this plan is essentially complete with assignments of the ground and first two torsional states accomplished through 1.6 THz. The ground and first torsional state are fit to near experimental uncertainty. The application of this approach to methyl formate, for which a similar data set has been compiled[e], will also be discussed.

[a] Pickett HM. J. Mol. Spec. 1991; 148(2): 371-377.
[b] Pickett HM, *et al.*, J. Quant. Spectrosc. Radiat. Transfer. 1998; 60(5), 883-890.
[c] Müller HSP, Schlöder F, Stutzki J, Winnewisser G. J. Mol. Struct. 2005; 742: 215-227.
[d] Kleiner, Lovas & Godefroid, J. Phys. Chem. Ref. Data. 1996, Vol 25(4).
[e] Carvajal M, *et al.*, J. Mol. Spec. 2007; 246(2), 158-166.