

P4944: A Microwave and Computational Study of Acid Anhydrides

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- Need for automated spectral assignment has been established and prior auto-programs acknowledged
- DAPPERS progression based intelligent assignment algorithm has been explored
- Special focus given to the algorithm's speed and accuracy
- Additional DAPPERS features presented:
 - Graphical Peak Finder
 - Pickett .CAT file generator
 - Quantum Filters (progression selection menus)
- Success with Leopold and other rotational spectra has been presented



Spectra Assigned from Leopold Lab:

- trimethylammonium triflate
- trifluoroacetic anhydride (TFAA)
- TFAA monohydrate
- pivalic anhydride
- pivalic trifluoroacetic anhydride
- benzoic trifluoroacetic anhydride
- acetic trifluoroacetic anhydride A state
- acetic pivalic anhydride A state
- acetic anhydride AA state
- trifluoroacetic acid–trimethylamine