MICROWAVE SPECTRA AND STRUCTURE OF PIVALIC ANHYDRIDE $(CH_3)_3CCOOCOC(CH_3)_3$, AND PIVALIC - TRIFLUOROACETIC ANHYDRIDE $(CH_3)_3CCOOCOCF_3$

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Microwave spectra of pivalic anhydride ($(CH_3)_3CCOOCOC(CH_3)_3$) and pivalic – trifluoroacetic anhydride ($(CH_3)_3CCOOCOCF_3$) have been observed by chirped-pulse and cavity Fourier transform microwave spectroscopy. For pivalic anhydride, eight isotopologues corresponding to substitution on each atom in the heavy atom frame have been observed. For the pivalic – trifluoroacetic anhydride, ten isotopologues have been analyzed, and Kraitchman analyses provide accurate structural information about the heavy atom frame for both systems. The results indicate that the carbonyl groups are not coplanar, but rather, form dihedral angles of $53.9(39)^\circ$ in pivalic anhydride and $46.5(16)^\circ$ in pivalic – trifluoroacetic anhydride. These results are in good agreement with M06-2X/6-311++G(3df,3pd) calculations. Calculations at the same level indicate that the barriers to the carbonyl groups twisting through a planar configuration are 1.7 kcal/mol and 0.7 kcal/mol for pivalic and pivalic - trifluoroacetic anhydrides, respectively. Spectra for both forms of the parent species were assigned and fit in under five minutes using the new rotational spectral fitting program DAPPERS, and a brief synopsis of the process will be presented. A straightforward synthesis for the mixed pivalic – trifluoroacetic anhydride, which should be applicable to other anhydrides, will also be described.