THE MILLIMETER-WAVE ROTATIONAL SPECTRA OF PYRUVIC ACID AND OF GLYCOLIC ACID

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The two simple acids, 10-atom pyruvic acid ($CH_3COCOOH$) and 9-atom glycolic acid ($CH_2OHCOOH$), are candidate interstellar molecules and accurate knowledge of their rotational spectra is required prior to any radioastronomical searches. Previous studies of the most stable conformers of pyruvic acid[a] and of glycolic acid[b] were limited to the centimeter-wave rotational spectrum and those have now been extended to over 310 GHz.

Both molecules give rise to complex mm-wave rotational spectra due to satellites of low frequency vibrational modes. In the case of pyruvic acid the complexity is increased also by internal rotation splitting from the methyl torsion. We have successfully dealt with the analysis of the spectra by using the $AABS$ package for $Assignment\ and\ Analysis\ of\ Broadband\ Spectra$,[c] and several different fitting programs that have been made available to the spectroscopic community. The data also allow a comparison of the relative merits of three different programs for fitting internal rotation to experimental accuracy.[d]

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[a] R.Meyer and A.Bauder, $J.\ Mol.\ Spectrosc.$, **94**, 136-149 (1982), and references cited therein.

[b] C.E.Blom and A.Bauder, $Chem.\ Phys.\ Lett.$, **82**, 492-495 (1981).

[c] Z.Kisiel, PROSPE - Programs for ROtational SPEctroscopy, http://info.ifpan.edu.pl/~kisiel/prospe.htm

[d] Z.Kisiel, et al., $J.\ Mol.\ Spectrosc.$, **241**, 220-229 (2007).