PROPANE ISOTOPOLOGUES: HIGH RESOLUTION FAR-IR SYNCHROTRON SPECTRA OF PROPANE-D7 (CD3-CDH-CD3) AND PROPANE-D5 (CH3-CD2-CD3)

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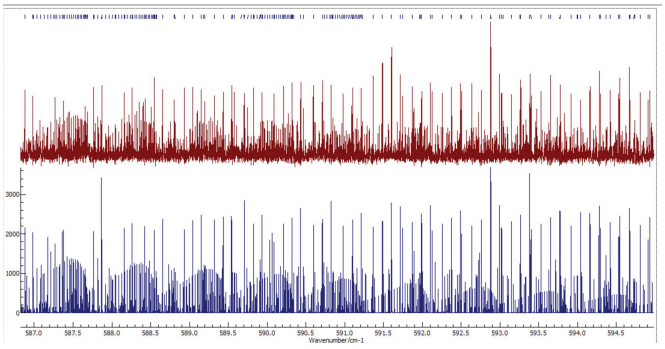

We continue our project of recording spectra and ro-ibrational analyses of propane isotopologues to determine ro-vibrational constants for this family of molecules. No MW, mm or sub-mm studies exist as of yet. IR/R spectra of propane-D_5 do not appear to have ever been reported on in the literature. There are only low/medium resolution data on the -D_7 species.[b] We acquired survey and high resolution (0.002-0.00096 cm^{-1}) synchrotron IR data at the CLS facility in Saskatoon for the -D_5 bands. We also now have preliminary values of its rotational constants from the B-type CCC bending mode near 332.7 cm^{-1}. For the -D_7 species we have preliminary analyses of the B-type ν_{14}(A') CCC bend near 305.24 $\mathrm{cm}^{-1}$and the ν_{13} (A') C-type band near 579.34 cm^{-1}. The figure at the left is a part of the R-side of the ν_{13} band for Propane-D_7. Observed spectrum taken at 0.00096cm^{-1}resolution plotted above the PGOPHER[c] simulation.

[a]Deceased 21- September-2021

[b]Gough, Murphy and Raghavachari, J.Chem. Phys. 87, 3332 (1987) and refs. therein

[c]C. M. Western, B. E. Billinghurst PCCP 21, 13986 (2019) and refs. therein.