FIRST HIGH RESOLUTION IR SPECTRA OF 2,2-D_2-PROPANE. THE ν_{15} (B_1) A-TYPE BAND NEAR 954.709 cm^{-1}. DETERMINATION OF GROUND AND UPPER STATE CONSTANTS.

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As part of our project on the study of isotopologues of propane we have taken the spectra of the 2-D and 2,2-D_2 substituted species. There have been no studies of these species since the early IR studies. [a] [b] [c] [d]

We recorded high resolution ($\Delta\nu$ = 0.0009 cm^{-1}) FTS data on the Canadian Light Source Far-IR beamline. The spectra of all bands of both species in the region examined (500 - 1250 cm^{-1}) show torsionally perturbed lines, all but one band appearing globally perturbed. Virtually all bands were not amenable to analysis at present except for the ν_{15} (B_1) A-type band centered at 954.709 cm^{-1}. One can still see a few perturbed lines with torsional components but overall most lines were single and could be readily assigned using traditional methods. The spectrum is modelled well using PGOPHER.[e] No MW determined GS constants were available so we have analyzed about 3500 levels to determine both ground state and upper state rotational constants.

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[a] Friedman & Turkevich, J. Chem. Phys. **17**, 1012 ff. (1949); McMurry, Thornton & Condon, J. Chem. Phys. **17**, 918 ff. (1949).

[b] McMurry & Thornton, J. Chem. Phys. **19**, 1014 ff.(1951).

[c] Gayles & King, Spectrochim. Acta **21**, 543 ff.(1965).

[d] Kondo & Saeki, Spectrochim. Acta **29A**, 735 ff. (1973).

[e] Western, J. Quant. Spectrosc. Rad. Transf. **186**, 221 ff. (2017).