PROPANE ISOTOPOLOGUES: HIGH RESOLUTION SYNCHROTRON FAR-IR SPECTRA OF THE SYMMETRICALLY DEUTERATED SPECIES $CH_3CH_2CD_3$, $CD_3CH_2CD_3$ AND C_3D_8. FIRST EXPERIMENTALLY DETERMINED GROUND STATE CONSTANTS FOR THESE SPECIES

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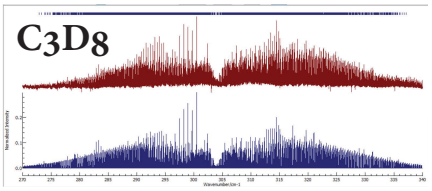

We are continuing our project of obtaining high resolution vibration-rotation spectra of propane isotopologues using the Far-IR beamline at the Canadian National Synchrotron (CLS). We have already reported on all the singly ^{13}C and singly D substituted varieties as well as the 2,2-D_2 species at previous ISMS meetings (2017-19) and in a recent paper on 2-^{13}C-Propane [a]. These studies have allowed us to determine ground state inertial and centrifugal distortion rotational constants for these molecules that have no pure rotational spectra in the literature except for the 6 lines reported by Lide[b] in 1960 of normal propane and two ^{13}C and D versions. In this talk we will present the high resolution spectra (0.00096 cm^{-1}) for the CCC skeletal bendings of $CH_3CH_2CD_3$, $CD_3CH_2CD_3$ and C_3D_8. These studies have yielded corrected observed band origins[c] and rotational constants for the three species. Preliminary values for each species are listed here in wavenumbers. $CH_3CH_2CD_3$: ν_9 = 335.664740(40), A_0 = 0.8185513(12), B_0 = 0.24400666(39), C_0 = 0.21852642(41); $CD_3CH_2CD_3$: ν_{16} = 306.4, A_0 = 0.711202, B_0 = 0.213021, C_0 = 0.193244; C_3D_8: ν_9 = 303.936065(23), A_0 = 0.58742224(42), B_0 = 0.20872437(23), C_0 = 0.18588200(18).

[a] Daunt, Grzywacz, Western, Lafferty, Flaud, Billinghurst, and Hutchings, J. Mol. Structure, in press (doi:10.1016/j.molstruc.2020.127851).

[b] D. R. Lide, J. Chem. Physics 33, 1514-1518 (1960).

[c] Gayles and King, Spectrochim. Acta 21, 543-557 (1965); K. M. Gough, W. F. Murphy and K. Raghavachari, J. Chem. Phys. 87, 3332-3340 (1987).